



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:20 PM UTC

PDB ID : 7V28 / pdb_00007v28
Title : Crystal Structure of phthalate dioxygenase in complex with terephthalate
Authors : Mahto, J.K.; Kumar, P.
Deposited on : 2021-08-07
Resolution : 3.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

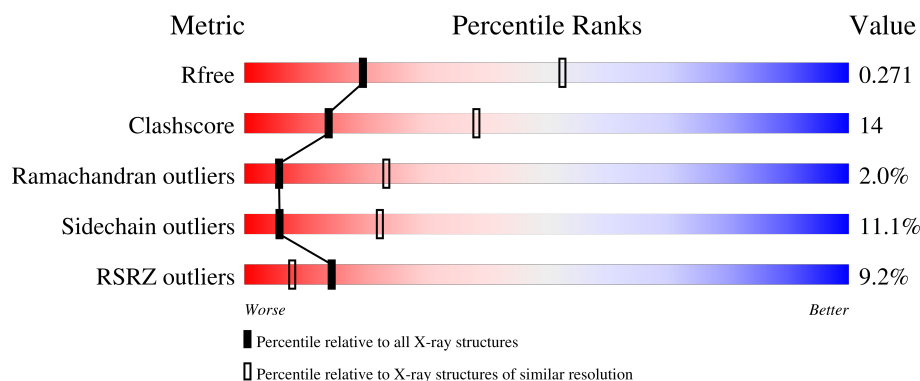
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	4% 59% 26% 7% 8%
1	B	439	8% 64% 28% . .
1	C	439	7% 58% 30% 5% 7%
1	D	439	5% 57% 30% 5% 8%
1	E	439	15% 58% 31% . 7%

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Mol	Chain	Length	Quality of chain
1	F	439	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	D	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19601 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

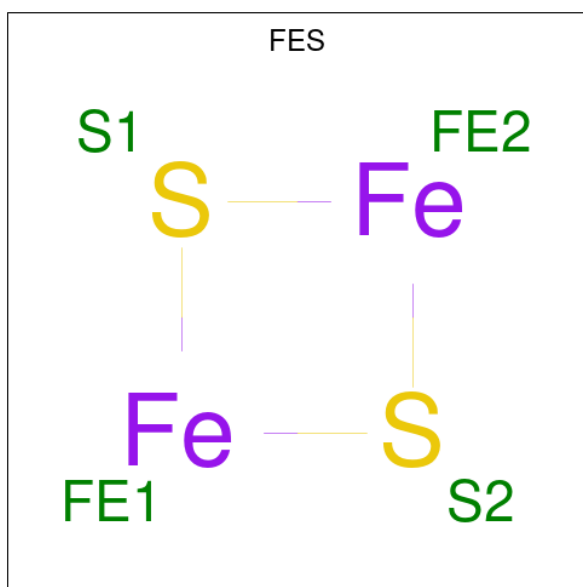
- Molecule 1 is a protein called Rieske (2Fe-2S) domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3192	2011	564	593	24			
1	B	425	Total	C	N	O	S	0	0	0
			3335	2100	590	621	24			
1	C	407	Total	C	N	O	S	0	0	0
			3202	2017	566	595	24			
1	D	404	Total	C	N	O	S	0	0	0
			3186	2008	563	591	24			
1	E	407	Total	C	N	O	S	0	0	0
			3202	2017	566	595	24			
1	F	406	Total	C	N	O	S	0	0	0
			3194	2012	565	594	23			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

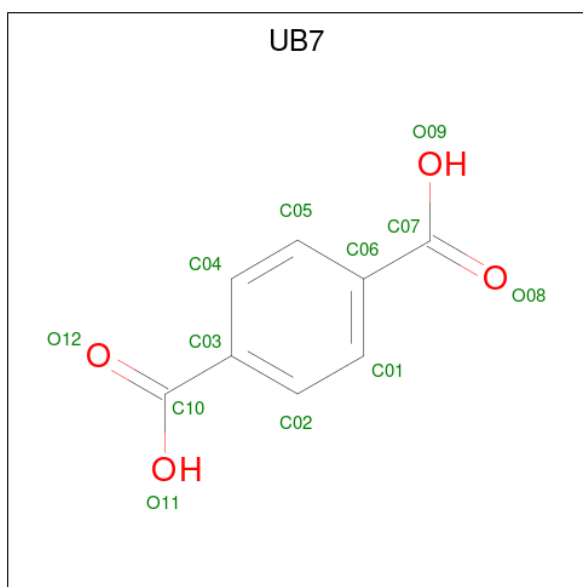
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is terephthalic acid (CCD ID: UB7) (formula: $C_8H_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	8	4		

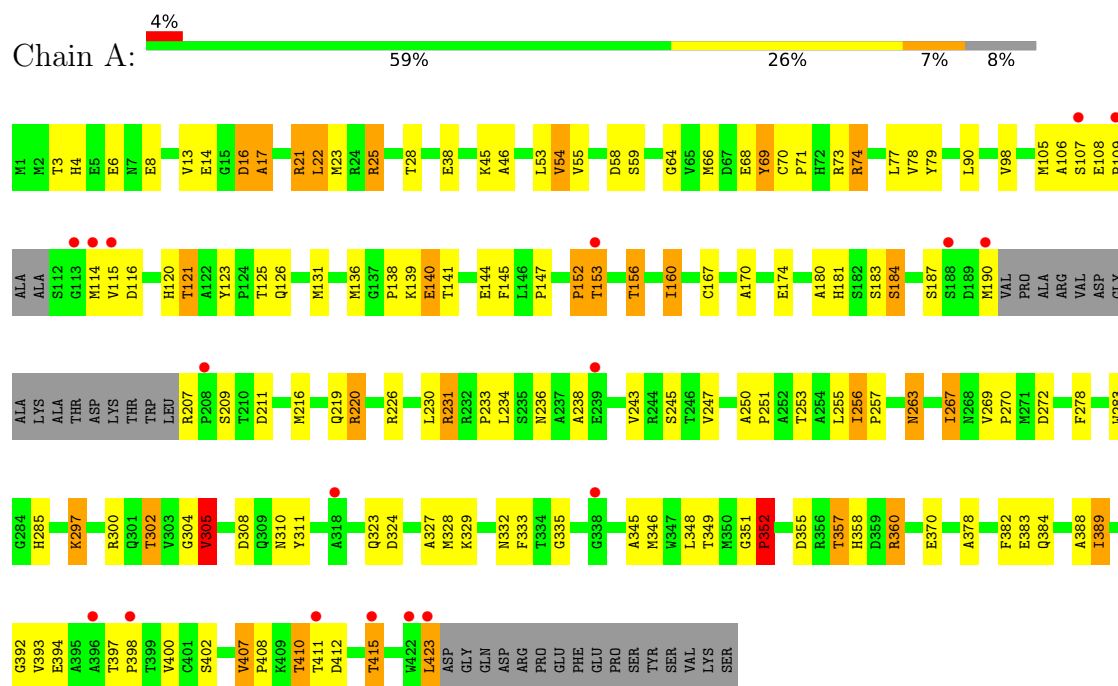
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	41	Total	O	0	0
			41	41		
5	C	41	Total	O	0	0
			41	41		
5	D	43	Total	O	0	0
			43	43		
5	E	40	Total	O	0	0
			40	40		
5	F	36	Total	O	0	0
			36	36		

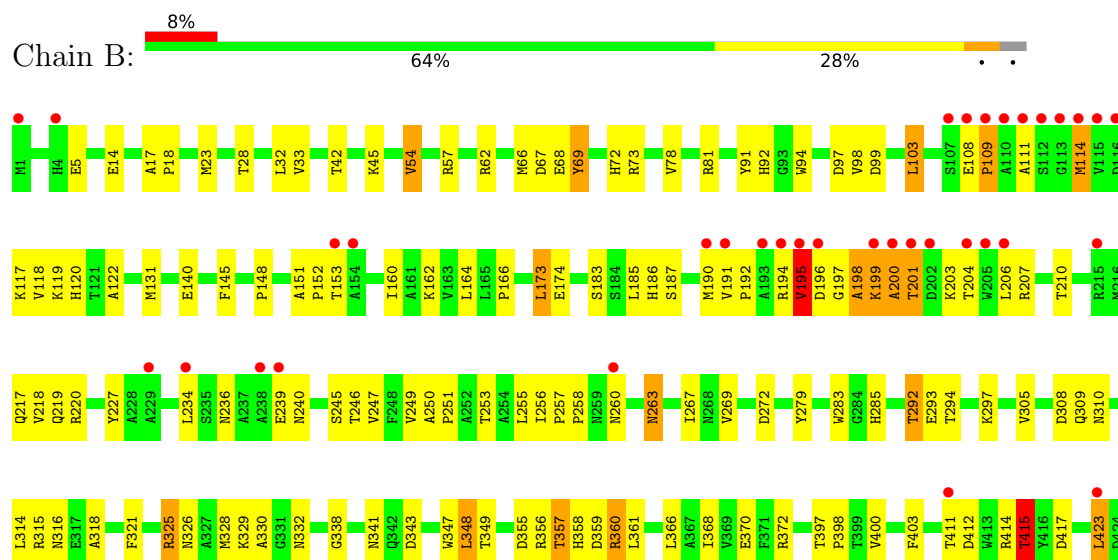
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Rieske (2Fe-2S) domain protein



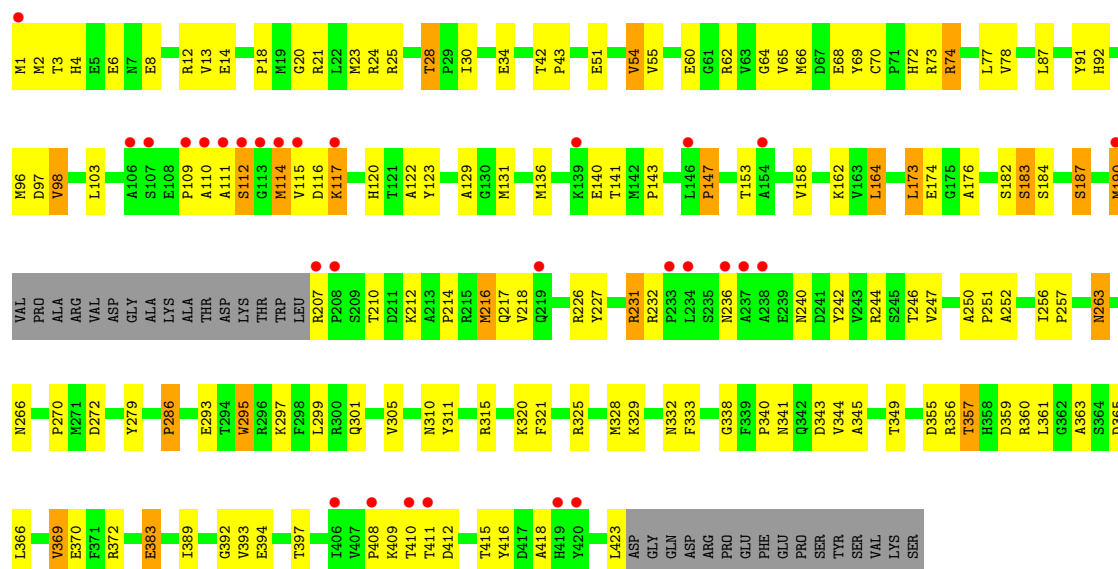
• Molecule 1: Rieske (2Fe-2S) domain protein



Q425
GLN
ASP
ARG
PRO
GLU
PHE
GLU
PRO
TYR
SER
VAL
LYS
SER

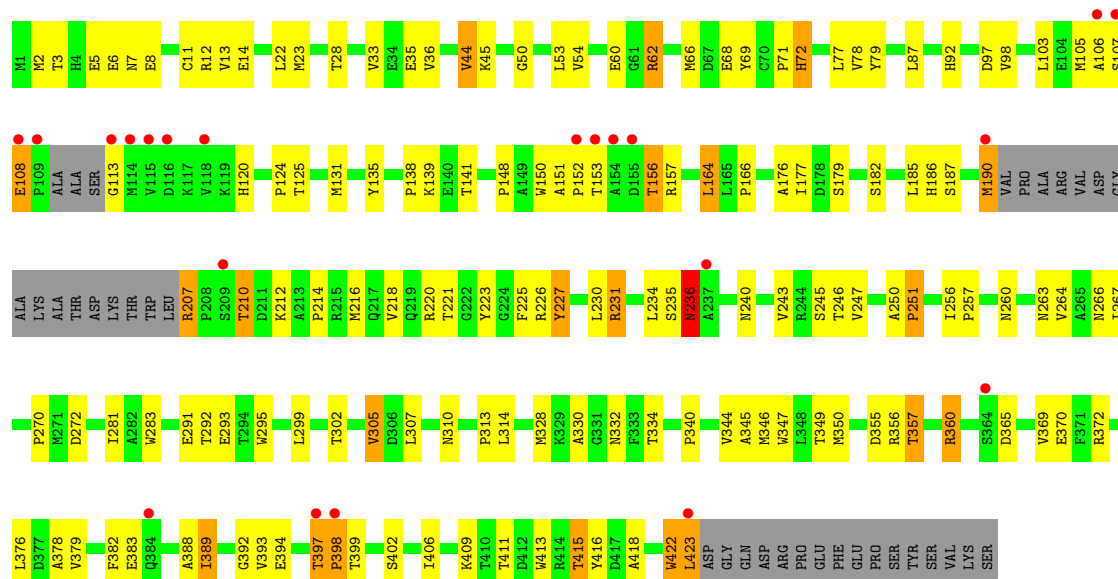
• Molecule 1: Rieske (2Fe-2S) domain protein

Chain C: 7% 58% 30% 5% 7%



• Molecule 1: Rieske (2Fe-2S) domain protein

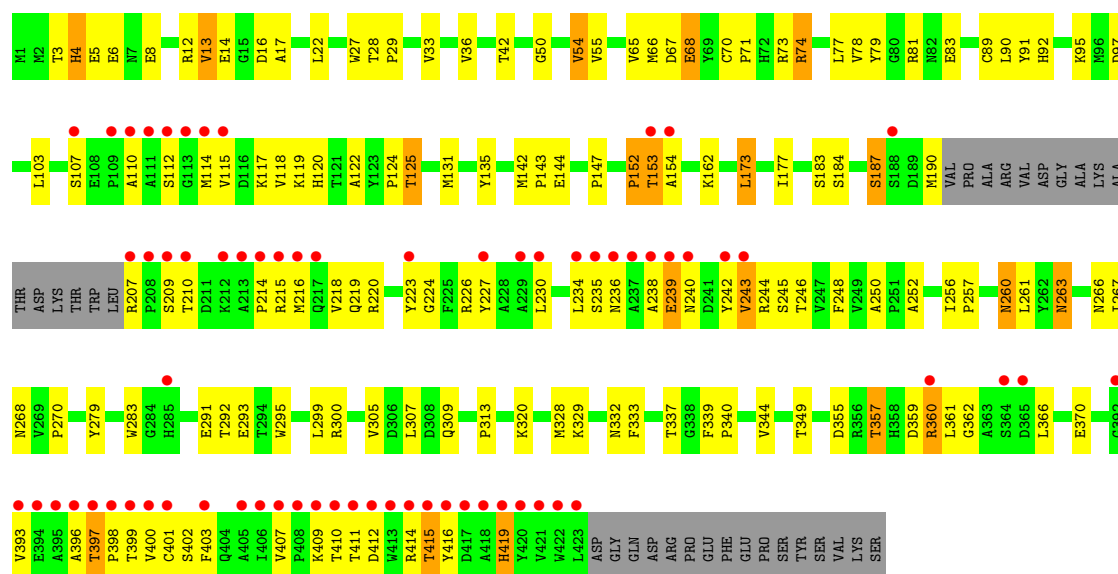
Chain D: 5% 57% 30% 5% 8%



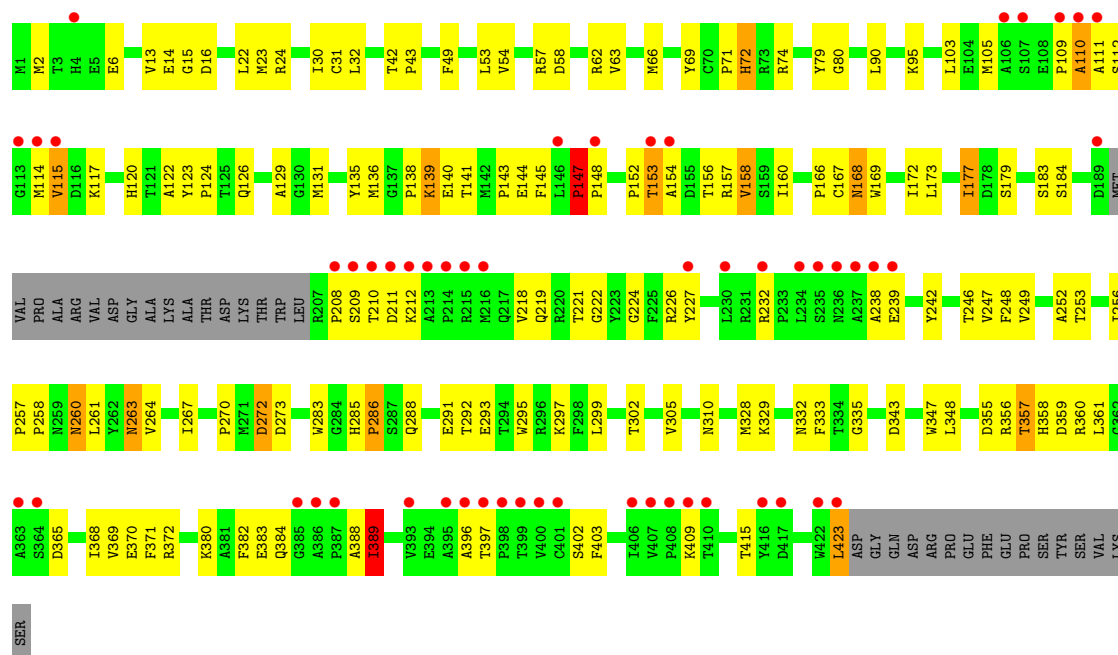
• Molecule 1: Rieske (2Fe-2S) domain protein

Chain E: 15% 58% 31% 7%





• Molecule 1: Rieske (2Fe-2S) domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.25Å 122.67Å 163.50Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	160.43 – 3.07 160.43 – 3.07	Depositor EDS
% Data completeness (in resolution range)	97.6 (160.43-3.07) 97.6 (160.43-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.266 0.215 , 0.271	Depositor DCC
R_{free} test set	3161 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	19601	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, FES, UB7

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/3278	1.12	10/4462 (0.2%)
1	B	0.53	0/3426	1.13	4/4668 (0.1%)
1	C	0.53	0/3289	1.12	4/4479 (0.1%)
1	D	0.53	0/3272	1.12	2/4454 (0.0%)
1	E	0.53	0/3289	1.09	5/4479 (0.1%)
1	F	0.52	0/3281	1.11	3/4469 (0.1%)
All	All	0.53	0/19835	1.12	28/27011 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	VAL	N-CA-C	-7.26	106.02	112.12
1	A	304	GLY	CA-C-N	-6.96	115.46	122.77
1	A	304	GLY	C-N-CA	-6.96	115.46	122.77
1	F	147	PRO	N-CA-C	6.93	119.16	110.70
1	C	28	THR	CA-CB-OG1	-6.55	99.77	109.60
1	E	337	THR	CB-CA-C	6.28	120.09	109.80
1	A	69	TYR	CB-CA-C	6.26	120.68	110.22
1	F	69	TYR	CB-CA-C	6.09	119.79	109.80
1	B	69	TYR	CB-CA-C	6.08	119.78	109.80
1	B	423	LEU	N-CA-C	-6.06	107.71	114.62
1	C	69	TYR	CB-CA-C	6.05	119.72	109.80
1	A	116	ASP	CB-CA-C	-5.99	101.22	110.81
1	F	310	ASN	CB-CA-C	-5.93	101.41	111.02
1	A	352	PRO	N-CA-CB	-5.75	97.21	103.25
1	A	308	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	147	PRO	N-CA-C	5.37	117.25	110.70
1	A	410	THR	CB-CA-C	5.21	119.06	109.99
1	A	278	PHE	CA-CB-CG	5.18	118.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	ARG	CG-CD-NE	-5.18	100.61	112.00
1	E	210	THR	CB-CA-C	5.17	118.07	111.40
1	B	415	THR	CA-CB-OG1	-5.13	101.91	109.60
1	D	166	PRO	CB-CA-C	-5.09	105.68	112.97
1	D	251	PRO	N-CD-CG	-5.08	97.71	103.80
1	B	42	THR	CB-CA-C	-5.07	101.24	109.56
1	E	68	GLU	CB-CG-CD	5.04	121.18	112.60
1	E	67	ASP	CA-C-N	5.03	127.01	120.28
1	E	67	ASP	C-N-CA	5.03	127.01	120.28
1	A	58	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3192	0	3073	81	0
1	B	3335	0	3217	90	0
1	C	3202	0	3084	99	0
1	D	3186	0	3068	105	0
1	E	3202	0	3084	94	0
1	F	3194	0	3075	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	4	0	0	2	0
3	E	4	0	0	1	0
3	F	4	0	0	1	0
4	B	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	47	0	0	2	0
5	B	41	0	0	0	0
5	C	41	0	0	3	0
5	D	43	0	0	5	0
5	E	40	0	0	6	0
5	F	36	0	0	0	0
All	All	19601	0	18601	548	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:ARG:HG3	1:E:360:ARG:HH11	1.00	1.17
1:D:60:GLU:HG3	1:D:62:ARG:NH1	1.66	1.11
1:D:360:ARG:HG3	1:D:360:ARG:HH11	1.17	1.07
1:C:218:VAL:HG11	1:C:370:GLU:HG2	1.39	1.00
1:D:230:LEU:HD23	1:D:243:VAL:HG22	1.42	0.98
1:C:231:ARG:HH11	1:C:231:ARG:CG	1.78	0.95
1:C:231:ARG:HH11	1:C:231:ARG:HG2	1.29	0.94
1:E:218:VAL:HG11	1:E:370:GLU:HG2	1.47	0.94
1:F:183:SER:HB3	1:F:212:LYS:HG2	1.50	0.94
1:B:360:ARG:HG3	1:B:360:ARG:HH11	1.35	0.92
1:F:173:LEU:HD13	1:F:252:ALA:HA	1.51	0.92
1:D:378:ALA:HB1	1:D:389:ILE:HG21	1.53	0.91
1:B:66:MET:HE3	1:B:120:HIS:HD2	1.37	0.89
1:C:217:GLN:O	1:C:227:TYR:HB2	1.72	0.89
1:E:360:ARG:HG3	1:E:360:ARG:NH1	1.75	0.88
1:B:397:THR:HB	1:B:398:PRO:CD	2.04	0.86
1:C:54:VAL:HG22	1:C:68:GLU:HA	1.58	0.86
1:D:383:GLU:HG2	5:D:609:HOH:O	1.75	0.85
1:D:392:GLY:HA3	5:D:622:HOH:O	1.75	0.84
1:D:378:ALA:HB1	1:D:389:ILE:CG2	2.06	0.84
1:C:14:GLU:OE2	1:C:272:ASP:HB2	1.76	0.83
1:D:60:GLU:CG	1:D:62:ARG:NH1	2.41	0.83
1:F:355:ASP:OD1	1:F:357:THR:HB	1.77	0.83
1:D:256:ILE:HB	1:D:264:VAL:HG12	1.61	0.82
1:F:227:TYR:CE1	1:F:246:THR:HB	2.15	0.82
1:D:220:ARG:HD3	1:D:370:GLU:OE2	1.79	0.81
1:E:397:THR:HB	1:E:398:PRO:CD	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:ARG:HH11	1:E:360:ARG:CG	1.88	0.78
1:E:407:VAL:HG21	1:E:416:TYR:HE1	1.48	0.78
1:F:261:LEU:HD23	1:F:288:GLN:HG2	1.66	0.78
1:D:378:ALA:CB	1:D:389:ILE:HG21	2.14	0.78
1:C:110:ALA:HB1	1:C:115:VAL:HG11	1.64	0.77
1:E:397:THR:HB	1:E:398:PRO:HD3	1.67	0.77
1:D:360:ARG:HH11	1:D:360:ARG:CG	1.98	0.77
1:D:356:ARG:HG2	1:D:372:ARG:NH2	2.00	0.76
1:B:315:ARG:HB3	1:B:321:PHE:HA	1.68	0.76
1:D:347:TRP:HA	1:D:350:MET:HE3	1.66	0.76
1:F:126:GLN:HG2	1:F:145:PHE:CD2	2.21	0.75
1:B:185:LEU:HD23	1:B:186:HIS:CE1	2.22	0.75
1:D:231:ARG:HG2	1:D:231:ARG:HH11	1.51	0.75
1:F:173:LEU:CD1	1:F:252:ALA:HA	2.16	0.75
1:C:112:SER:HB3	5:C:623:HOH:O	1.87	0.74
1:C:412:ASP:O	1:C:415:THR:HG22	1.88	0.74
1:D:295:TRP:CE2	1:D:299:LEU:HD11	2.22	0.74
1:A:397:THR:HB	1:A:398:PRO:CD	2.17	0.74
1:B:217:GLN:O	1:B:227:TYR:HB2	1.87	0.74
1:B:397:THR:HB	1:B:398:PRO:HD3	1.69	0.74
1:F:258:PRO:HB3	1:F:263:ASN:HA	1.69	0.73
1:C:20:GLY:O	1:C:24:ARG:HG3	1.89	0.72
1:B:54:VAL:HG22	1:B:68:GLU:HA	1.71	0.72
1:F:184:SER:O	1:F:333:PHE:CE2	2.43	0.71
1:F:226:ARG:HG2	1:F:247:VAL:HG22	1.71	0.71
1:D:302:THR:HB	1:D:305:VAL:HG13	1.73	0.70
1:A:108:GLU:HG3	1:A:109:PRO:HD2	1.74	0.70
1:D:60:GLU:CG	1:D:62:ARG:HH11	2.04	0.70
1:E:184:SER:O	1:E:187:SER:HB2	1.91	0.70
1:F:124:PRO:HG2	1:F:135:TYR:HB3	1.74	0.70
1:E:407:VAL:HG21	1:E:416:TYR:CE1	2.27	0.69
1:A:231:ARG:HH11	1:A:231:ARG:HG2	1.58	0.69
1:D:60:GLU:HG3	1:D:62:ARG:HH11	1.55	0.69
1:D:156:THR:HG23	1:D:422:TRP:HZ3	1.57	0.69
1:C:256:ILE:HG23	1:C:257:PRO:HD2	1.74	0.69
1:F:153:THR:HG22	1:F:154:ALA:H	1.58	0.68
1:B:219:GLN:HE21	1:B:414:ARG:HD2	1.58	0.68
1:B:66:MET:CE	1:B:120:HIS:HD2	2.06	0.68
1:D:60:GLU:HG3	1:D:62:ARG:HH12	1.52	0.68
1:A:14:GLU:OE2	1:A:272:ASP:HB2	1.92	0.68
1:A:147:PRO:HB3	1:A:152:PRO:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:VAL:HG22	1:E:68:GLU:HA	1.74	0.68
1:A:4:HIS:O	1:A:8:GLU:HG2	1.93	0.67
1:A:382:PHE:C	1:A:384:GLN:H	2.02	0.67
1:C:416:TYR:CE2	1:C:418:ALA:HB2	2.29	0.67
1:C:60:GLU:HG2	1:C:62:ARG:HH11	1.59	0.67
1:C:226:ARG:HG2	1:C:247:VAL:HG22	1.76	0.67
1:D:92:HIS:HB2	3:D:502:FES:S1	2.35	0.67
1:E:220:ARG:HD3	1:E:370:GLU:OE2	1.94	0.67
1:F:285:HIS:CD2	1:F:423:LEU:HD12	2.30	0.67
1:A:140:GLU:CD	1:A:140:GLU:H	2.03	0.66
1:D:355:ASP:OD1	1:D:357:THR:HB	1.94	0.66
1:B:219:GLN:NE2	1:B:414:ARG:HD2	2.11	0.66
1:D:299:LEU:HB3	1:D:340:PRO:HG2	1.78	0.66
1:C:263:ASN:HB3	5:C:601:HOH:O	1.96	0.66
1:C:173:LEU:HD13	1:C:252:ALA:HA	1.76	0.66
1:E:263:ASN:HB2	1:E:283:TRP:NE1	2.11	0.66
1:B:66:MET:HG2	1:B:122:ALA:HB2	1.77	0.65
1:F:109:PRO:C	1:F:111:ALA:H	2.05	0.65
1:E:73:ARG:O	1:E:74:ARG:HB2	1.96	0.65
1:E:359:ASP:HB3	1:E:361:LEU:HD21	1.78	0.65
1:C:231:ARG:CG	1:C:231:ARG:NH1	2.49	0.65
1:A:220:ARG:NH1	1:A:370:GLU:OE2	2.30	0.64
1:B:285:HIS:CD2	1:B:423:LEU:HD12	2.32	0.64
1:D:14:GLU:OE2	1:D:272:ASP:HB2	1.98	0.64
1:A:170:ALA:O	1:A:174:GLU:HG3	1.98	0.64
1:A:302:THR:HB	1:A:305:VAL:HG13	1.80	0.64
1:B:227:TYR:CE1	1:B:246:THR:HB	2.33	0.63
1:B:368:ILE:O	1:B:372:ARG:HG3	1.98	0.63
1:D:7:ASN:O	1:D:11:CYS:HB2	1.98	0.63
1:F:343:ASP:HB3	1:F:347:TRP:CZ2	2.34	0.63
1:B:236:ASN:O	1:B:240:ASN:HB2	1.99	0.62
1:E:235:SER:O	1:E:236:ASN:HB2	1.98	0.62
1:E:239:GLU:HG2	1:E:239:GLU:O	1.98	0.62
1:E:242:TYR:OH	1:E:244:ARG:NH2	2.32	0.62
1:D:397:THR:HB	1:D:398:PRO:HD2	1.80	0.62
1:F:14:GLU:OE2	1:F:272:ASP:HB2	1.98	0.62
1:D:179:SER:O	1:D:231:ARG:NH2	2.32	0.62
1:F:57:ARG:NH1	1:F:63:VAL:HG23	2.14	0.62
1:D:14:GLU:HG2	1:D:50:GLY:HA3	1.82	0.61
1:A:355:ASP:OD1	1:A:357:THR:HB	2.00	0.61
1:B:66:MET:HE3	1:B:120:HIS:CD2	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ALA:HB2	1:D:330:ALA:HB2	1.82	0.61
1:C:227:TYR:CE1	1:C:246:THR:HB	2.35	0.61
1:E:300:ARG:HD2	5:E:605:HOH:O	2.00	0.61
1:F:382:PHE:C	1:F:384:GLN:H	2.07	0.61
1:A:360:ARG:HB2	1:E:71:PRO:O	2.01	0.61
1:C:184:SER:O	1:C:187:SER:HB3	2.00	0.61
1:B:360:ARG:HG3	1:B:360:ARG:NH1	2.10	0.61
1:F:227:TYR:HE1	1:F:246:THR:HB	1.64	0.61
1:B:54:VAL:HG13	1:B:78:VAL:HG22	1.83	0.60
1:F:261:LEU:CD2	1:F:288:GLN:HG2	2.31	0.60
1:A:66:MET:HE3	1:A:120:HIS:HD2	1.66	0.60
1:B:92:HIS:HB2	3:B:502:FES:S1	2.42	0.60
1:D:131:MET:HE1	1:D:281:ILE:HD11	1.83	0.59
1:A:73:ARG:O	1:A:74:ARG:HB2	2.02	0.59
1:B:343:ASP:HB3	1:B:347:TRP:CZ2	2.37	0.59
1:C:2:MET:HE3	1:C:6:GLU:HB3	1.85	0.59
1:C:114:MET:HA	1:C:117:LYS:HB2	1.83	0.59
1:F:57:ARG:HH11	1:F:57:ARG:HG3	1.67	0.59
1:B:131:MET:HE3	1:B:160:ILE:HD13	1.85	0.59
1:F:285:HIS:HD2	1:F:423:LEU:HD12	1.67	0.59
1:D:156:THR:HG23	1:D:422:TRP:CZ3	2.37	0.59
1:A:70:CYS:HB2	1:A:77:LEU:HD21	1.83	0.59
1:D:423:LEU:HA	5:D:636:HOH:O	2.03	0.58
1:C:55:VAL:HG13	1:C:65:VAL:HG22	1.85	0.58
1:C:54:VAL:HG13	1:C:78:VAL:HG22	1.86	0.58
1:D:105:MET:O	1:D:107:SER:N	2.35	0.58
1:C:176:ALA:HB2	1:C:266:ASN:HD22	1.68	0.58
1:E:124:PRO:HG2	1:E:135:TYR:HB3	1.86	0.58
1:E:14:GLU:HG2	1:E:50:GLY:HA3	1.86	0.58
1:C:231:ARG:HG2	1:C:231:ARG:NH1	2.08	0.58
1:F:359:ASP:HB3	1:F:361:LEU:HD21	1.86	0.57
1:D:230:LEU:CD2	1:D:243:VAL:HG22	2.24	0.57
1:C:60:GLU:CG	1:C:62:ARG:HH11	2.18	0.57
1:E:13:VAL:HG21	1:E:270:PRO:HB2	1.85	0.57
1:F:168:ASN:HB2	1:F:273:ASP:O	2.05	0.57
1:D:382:PHE:CD1	1:D:388:ALA:HB2	2.39	0.57
1:E:110:ALA:C	1:E:112:SER:H	2.11	0.57
1:C:231:ARG:HE	1:C:244:ARG:HD3	1.68	0.57
1:C:131:MET:HE2	1:C:279:TYR:CD1	2.40	0.57
1:D:345:ALA:O	1:D:349:THR:HG23	2.04	0.57
1:C:164:LEU:HD22	1:C:310:ASN:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:TYR:HE2	1:C:418:ALA:HB2	1.70	0.57
1:F:263:ASN:HB2	1:F:283:TRP:NE1	2.20	0.56
1:C:66:MET:HG2	1:C:122:ALA:HB2	1.85	0.56
1:B:66:MET:CE	1:B:120:HIS:CD2	2.87	0.56
1:B:166:PRO:HD2	1:B:348:LEU:HD21	1.86	0.56
1:E:66:MET:HE3	1:E:120:HIS:HD2	1.70	0.56
1:A:126:GLN:HG2	1:A:145:PHE:CD1	2.41	0.56
1:F:123:TYR:CD1	1:F:136:MET:HA	2.40	0.56
1:C:244:ARG:NH1	1:C:257:PRO:HB2	2.19	0.56
1:E:118:VAL:C	1:E:119:LYS:HE2	2.30	0.56
1:B:397:THR:HB	1:B:398:PRO:HD2	1.86	0.56
1:D:226:ARG:HG2	1:D:247:VAL:HG22	1.87	0.56
1:F:328:MET:HG3	1:F:335:GLY:HA3	1.88	0.55
1:A:219:GLN:OE1	1:A:226:ARG:NH1	2.39	0.55
1:A:54:VAL:HG22	1:A:68:GLU:HA	1.89	0.55
1:A:123:TYR:CE2	1:A:136:MET:HE3	2.42	0.55
1:D:97:ASP:HB3	1:D:103:LEU:HD11	1.87	0.55
1:B:355:ASP:OD1	1:B:357:THR:HB	2.06	0.55
1:F:239:GLU:O	1:F:239:GLU:HG2	2.06	0.55
1:B:174:GLU:HG2	1:B:368:ILE:HG23	1.88	0.55
1:E:407:VAL:HB	5:E:601:HOH:O	2.07	0.55
1:B:412:ASP:O	1:B:415:THR:HB	2.07	0.55
1:F:380:LYS:O	1:F:384:GLN:HG3	2.07	0.55
1:A:236:ASN:C	1:A:238:ALA:H	2.15	0.55
1:A:357:THR:HG22	1:A:358:HIS:ND1	2.22	0.55
1:A:408:PRO:C	1:A:410:THR:H	2.15	0.55
1:D:360:ARG:HG3	1:D:360:ARG:NH1	1.98	0.55
1:F:396:ALA:O	1:F:397:THR:HG23	2.07	0.55
1:E:309:GLN:HG2	5:E:636:HOH:O	2.07	0.54
1:F:126:GLN:HG2	1:F:145:PHE:CE2	2.42	0.54
1:B:195:VAL:HG21	1:B:206:LEU:HB3	1.89	0.54
1:D:182:SER:HB3	1:D:190:MET:HG3	1.90	0.54
1:A:247:VAL:HB	1:A:255:LEU:HD12	1.89	0.54
1:B:131:MET:HE2	1:B:279:TYR:CD1	2.43	0.54
1:E:8:GLU:OE2	1:E:12:ARG:NE	2.37	0.54
1:E:340:PRO:O	1:E:344:VAL:HG23	2.08	0.54
1:F:109:PRO:C	1:F:111:ALA:N	2.66	0.54
1:A:256:ILE:HG23	1:A:257:PRO:HD2	1.90	0.54
1:C:231:ARG:HH11	1:C:231:ARG:HG3	1.68	0.53
1:D:356:ARG:HG2	1:D:372:ARG:CZ	2.37	0.53
1:F:22:LEU:C	1:F:22:LEU:HD23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:TYR:CE2	1:E:349:THR:HG21	2.44	0.53
1:B:99:ASP:O	1:B:122:ALA:HB3	2.09	0.53
1:E:65:VAL:HG23	1:E:125:THR:HG21	1.91	0.53
1:A:394:GLU:OE2	1:A:394:GLU:HA	2.08	0.53
1:A:407:VAL:HG12	1:A:408:PRO:HD2	1.91	0.53
1:B:199:LYS:HG3	1:B:260:ASN:HD22	1.73	0.53
1:B:359:ASP:HB3	1:B:361:LEU:HD21	1.89	0.53
1:F:357:THR:HG22	1:F:358:HIS:ND1	2.23	0.53
1:A:211:ASP:HB3	1:A:231:ARG:HB3	1.90	0.53
1:B:108:GLU:OE2	1:C:363:ALA:N	2.42	0.53
1:D:393:VAL:HG13	1:D:394:GLU:HG2	1.91	0.53
1:A:323:GLN:HA	1:A:335:GLY:O	2.08	0.53
1:B:201:THR:H	1:B:203:LYS:H	1.56	0.53
1:B:256:ILE:HG23	1:B:257:PRO:HD2	1.90	0.53
1:E:214:PRO:HG2	1:E:216:MET:HE3	1.90	0.53
1:B:349:THR:HG21	1:F:79:TYR:HE2	1.73	0.52
1:C:140:GLU:CD	1:C:140:GLU:H	2.17	0.52
1:A:230:LEU:CD2	1:A:243:VAL:HG22	2.39	0.52
1:A:412:ASP:O	1:A:415:THR:HG22	2.09	0.52
1:B:397:THR:CB	1:B:398:PRO:CD	2.81	0.52
1:B:349:THR:HG21	1:F:79:TYR:CE2	2.45	0.52
1:C:218:VAL:HG11	1:C:370:GLU:CG	2.26	0.52
1:F:109:PRO:O	1:F:111:ALA:N	2.42	0.52
1:E:219:GLN:NE2	1:E:414:ARG:HD3	2.24	0.52
1:A:231:ARG:HH11	1:A:231:ARG:CG	2.21	0.52
1:A:346:MET:HA	1:A:346:MET:HE2	1.91	0.52
1:B:148:PRO:HG2	1:B:151:ALA:HB3	1.92	0.52
1:B:328:MET:HA	1:B:332:ASN:O	2.09	0.52
1:E:397:THR:CB	1:E:398:PRO:HD3	2.35	0.52
1:D:291:GLU:O	1:D:292:THR:C	2.53	0.52
1:D:124:PRO:HG2	1:D:135:TYR:HB3	1.92	0.52
1:E:263:ASN:HB2	1:E:283:TRP:CE2	2.45	0.52
1:F:131:MET:HE3	1:F:160:ILE:HD13	1.91	0.52
1:A:397:THR:HB	1:A:398:PRO:HD2	1.90	0.52
1:A:22:LEU:O	1:A:25:ARG:HB2	2.10	0.51
1:A:16:ASP:O	1:A:17:ALA:C	2.52	0.51
1:C:54:VAL:CG2	1:C:68:GLU:HA	2.37	0.51
1:C:218:VAL:HG23	1:C:366:LEU:CD2	2.40	0.51
1:D:236:ASN:O	1:D:240:ASN:HB2	2.10	0.51
1:E:328:MET:HA	1:E:332:ASN:O	2.10	0.51
1:A:230:LEU:HD23	1:A:243:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PHE:CD1	1:A:388:ALA:HB2	2.46	0.51
1:B:197:GLY:O	1:B:198:ALA:HB2	2.11	0.51
1:C:242:TYR:OH	1:C:244:ARG:NH2	2.43	0.51
1:C:345:ALA:O	1:C:349:THR:HG23	2.10	0.51
1:D:8:GLU:O	1:D:12:ARG:HG3	2.10	0.51
1:D:397:THR:HB	1:D:398:PRO:CD	2.40	0.51
1:A:382:PHE:C	1:A:384:GLN:N	2.69	0.51
1:B:109:PRO:C	1:B:111:ALA:H	2.17	0.51
1:C:173:LEU:O	1:C:174:GLU:C	2.54	0.51
1:D:235:SER:O	1:D:236:ASN:HB2	2.10	0.51
1:D:376:LEU:HA	1:D:379:VAL:HG12	1.93	0.51
1:F:382:PHE:CD1	1:F:388:ALA:HB2	2.46	0.51
1:A:54:VAL:HG13	1:A:78:VAL:HG22	1.91	0.51
1:C:218:VAL:CG1	1:C:370:GLU:HG2	2.28	0.51
1:D:150:TRP:CZ3	1:D:281:ILE:HD13	2.46	0.51
1:D:378:ALA:HB1	1:D:389:ILE:HG22	1.89	0.51
1:B:309:GLN:OE1	1:B:309:GLN:HA	2.10	0.51
1:E:339:PHE:CG	1:E:340:PRO:HD3	2.46	0.51
1:B:191:VAL:HG22	1:B:204:THR:OG1	2.11	0.50
1:A:153:THR:O	1:A:156:THR:OG1	2.28	0.50
1:A:53:LEU:HA	1:A:66:MET:O	2.11	0.50
1:B:32:LEU:HG	1:B:162:LYS:HD3	1.93	0.50
1:D:79:TYR:HE2	1:E:349:THR:HG21	1.76	0.50
1:A:16:ASP:O	1:A:21:ARG:NH1	2.45	0.50
1:E:401:CYS:SG	1:E:419:HIS:O	2.70	0.50
1:A:71:PRO:O	1:D:360:ARG:HB2	2.11	0.50
1:A:392:GLY:C	1:A:394:GLU:H	2.19	0.50
1:F:356:ARG:HD3	1:F:372:ARG:NE	2.26	0.50
1:C:70:CYS:HB2	1:C:77:LEU:HD21	1.93	0.50
1:B:210:THR:HG23	1:B:234:LEU:HD21	1.93	0.50
1:E:256:ILE:O	1:E:257:PRO:C	2.55	0.50
1:F:129:ALA:O	1:F:158:VAL:HG11	2.12	0.50
1:A:328:MET:HA	1:A:332:ASN:O	2.11	0.50
1:D:164:LEU:HD22	1:D:310:ASN:O	2.12	0.50
1:E:236:ASN:C	1:E:238:ALA:H	2.19	0.50
1:F:263:ASN:HB2	1:F:283:TRP:CE2	2.47	0.50
1:C:299:LEU:HD22	1:C:340:PRO:CG	2.41	0.49
1:D:72:HIS:HB3	3:D:502:FES:S2	2.52	0.49
1:C:183:SER:HB2	1:C:212:LYS:HG2	1.93	0.49
1:B:245:SER:HB3	1:B:403:PHE:CE2	2.48	0.49
1:C:24:ARG:HH21	1:C:136:MET:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LYS:HE3	1:C:311:TYR:CG	2.48	0.49
1:C:246:THR:OG1	1:C:257:PRO:HD3	2.13	0.49
1:F:218:VAL:CG1	1:F:219:GLN:N	2.76	0.49
1:F:295:TRP:CE2	1:F:299:LEU:HD11	2.47	0.49
1:E:226:ARG:HH21	1:E:403:PHE:HE2	1.60	0.49
1:B:360:ARG:HB2	1:F:71:PRO:O	2.12	0.49
1:B:97:ASP:HB3	1:B:103:LEU:HD11	1.95	0.49
1:D:231:ARG:HG2	1:D:231:ARG:NH1	2.24	0.49
1:C:23:MET:SD	1:C:270:PRO:HG3	2.52	0.49
1:E:27:TRP:HZ2	1:E:142:MET:HE3	1.78	0.49
1:C:328:MET:HA	1:C:332:ASN:O	2.13	0.49
1:D:397:THR:O	1:D:399:THR:N	2.45	0.49
1:A:263:ASN:HB2	1:A:283:TRP:CE2	2.47	0.49
1:C:21:ARG:HH12	1:C:383:GLU:HG2	1.78	0.49
1:E:97:ASP:OD2	1:E:97:ASP:C	2.55	0.49
1:D:148:PRO:HG2	1:D:151:ALA:HB3	1.95	0.49
1:E:66:MET:HG2	1:E:122:ALA:HB2	1.95	0.49
1:F:157:ARG:O	1:F:283:TRP:HA	2.13	0.49
1:A:126:GLN:HG2	1:A:145:PHE:CG	2.48	0.48
1:E:3:THR:OG1	1:E:6:GLU:HG3	2.13	0.48
1:F:285:HIS:CD2	1:F:423:LEU:CD1	2.96	0.48
1:E:295:TRP:CE2	1:E:299:LEU:HD11	2.48	0.48
1:A:131:MET:HE3	1:A:160:ILE:HD13	1.95	0.48
1:D:33:VAL:O	1:D:36:VAL:HG22	2.12	0.48
1:B:343:ASP:HB3	1:B:347:TRP:CH2	2.47	0.48
1:F:95:LYS:O	1:F:103:LEU:N	2.41	0.48
1:F:368:ILE:O	1:F:372:ARG:HG3	2.13	0.48
1:E:42:THR:HB	5:E:610:HOH:O	2.14	0.48
1:E:227:TYR:CE1	1:E:246:THR:HB	2.49	0.48
1:E:307:LEU:HD23	1:E:313:PRO:HA	1.95	0.48
1:B:173:LEU:O	1:B:173:LEU:HG	2.13	0.48
1:D:231:ARG:HH11	1:D:231:ARG:CG	2.24	0.48
1:B:195:VAL:HG11	1:B:206:LEU:HD13	1.95	0.48
1:C:236:ASN:HB2	5:C:637:HOH:O	2.13	0.48
1:C:293:GLU:OE1	1:C:293:GLU:HA	2.14	0.48
1:A:13:VAL:HG21	1:A:270:PRO:HB2	1.97	0.47
1:A:45:LYS:HG2	1:A:46:ALA:N	2.29	0.47
1:D:138:PRO:O	1:D:141:THR:OG1	2.31	0.47
1:E:173:LEU:HD13	1:E:252:ALA:HA	1.96	0.47
1:C:24:ARG:NH2	1:C:136:MET:HE2	2.29	0.47
1:E:184:SER:O	1:E:333:PHE:CE2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:VAL:HG21	1:C:270:PRO:HB2	1.97	0.47
1:C:92:HIS:HB2	3:C:502:FES:S2	2.55	0.47
1:F:291:GLU:O	1:F:292:THR:C	2.58	0.47
1:D:35:GLU:HB3	1:D:44:VAL:HG21	1.95	0.47
1:F:365:ASP:O	1:F:369:VAL:HG23	2.15	0.47
1:A:138:PRO:O	1:A:141:THR:OG1	2.30	0.47
1:D:210:THR:O	1:D:212:LYS:HG3	2.15	0.47
1:D:245:SER:O	1:D:402:SER:HB2	2.15	0.47
1:E:70:CYS:HB2	1:E:77:LEU:HD21	1.97	0.47
1:F:147:PRO:HA	1:F:148:PRO:HD2	1.86	0.47
1:B:94:TRP:HZ3	1:B:118:VAL:HG11	1.80	0.47
1:F:110:ALA:C	1:F:112:SER:H	2.23	0.47
1:F:218:VAL:HG12	1:F:219:GLN:N	2.30	0.47
1:A:25:ARG:HA	1:A:25:ARG:HD3	1.55	0.47
1:F:382:PHE:C	1:F:384:GLN:N	2.73	0.47
1:E:54:VAL:HG13	1:E:78:VAL:HG22	1.97	0.47
1:E:95:LYS:HE2	1:E:103:LEU:HD12	1.97	0.47
1:D:176:ALA:HB2	1:D:266:ASN:HD22	1.81	0.46
1:D:190:MET:HE3	1:D:207:ARG:NH1	2.30	0.46
1:F:173:LEU:HD22	1:F:371:PHE:CE1	2.50	0.46
1:A:333:PHE:O	1:E:81:ARG:NH1	2.48	0.46
1:D:372:ARG:O	1:D:376:LEU:HD12	2.16	0.46
1:E:22:LEU:HD23	1:E:22:LEU:C	2.39	0.46
1:A:236:ASN:C	1:A:238:ALA:N	2.72	0.46
1:C:190:MET:HE2	1:C:207:ARG:HH12	1.80	0.46
1:C:256:ILE:CG2	1:C:257:PRO:HD2	2.44	0.46
1:E:92:HIS:HB2	3:E:502:FES:S2	2.55	0.46
1:E:207:ARG:NH2	5:E:603:HOH:O	2.48	0.46
1:E:236:ASN:O	1:E:240:ASN:HB2	2.16	0.46
1:A:16:ASP:HB2	5:A:706:HOH:O	2.16	0.46
1:E:16:ASP:HB2	5:E:627:HOH:O	2.16	0.46
1:E:77:LEU:CD2	1:E:89:CYS:HB2	2.45	0.46
1:B:14:GLU:OE2	1:B:272:ASP:HB2	2.16	0.46
1:B:17:ALA:HA	1:B:18:PRO:HD3	1.80	0.46
1:C:2:MET:HE3	1:C:6:GLU:CB	2.46	0.46
1:E:74:ARG:HD2	1:E:74:ARG:HA	1.62	0.46
1:A:105:MET:O	1:A:107:SER:N	2.49	0.46
1:C:240:ASN:OD1	1:C:408:PRO:HA	2.16	0.46
1:C:299:LEU:HB3	1:C:340:PRO:HG2	1.98	0.46
1:F:256:ILE:HG23	1:F:257:PRO:HD2	1.97	0.46
1:A:397:THR:HB	1:A:398:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:THR:HG22	1:C:30:ILE:HD13	1.97	0.46
1:E:227:TYR:O	1:E:245:SER:HA	2.16	0.46
1:F:80:GLY:HA2	1:F:90:LEU:HG	1.98	0.46
1:C:301:GLN:HE22	1:C:341:ASN:CG	2.23	0.46
1:C:214:PRO:HG2	1:C:216:MET:HE3	1.98	0.45
1:A:184:SER:O	1:A:187:SER:OG	2.31	0.45
1:A:263:ASN:HB2	1:A:283:TRP:NE1	2.31	0.45
1:E:355:ASP:OD1	1:E:357:THR:HB	2.15	0.45
1:F:218:VAL:HG11	1:F:370:GLU:HG2	1.97	0.45
1:D:108:GLU:OE2	1:E:362:GLY:HA3	2.16	0.45
1:C:96:MET:SD	1:C:96:MET:N	2.89	0.45
1:C:129:ALA:HB1	1:C:158:VAL:HG11	1.98	0.45
1:A:297:LYS:O	1:A:300:ARG:HD3	2.16	0.45
1:C:355:ASP:OD1	1:C:357:THR:HB	2.17	0.45
1:C:190:MET:HE2	1:C:207:ARG:NH1	2.31	0.45
1:D:256:ILE:HG23	1:D:257:PRO:HD2	1.97	0.45
1:F:57:ARG:NH1	1:F:63:VAL:CG2	2.80	0.45
1:F:126:GLN:HG2	1:F:145:PHE:CG	2.51	0.45
1:B:164:LEU:HD22	1:B:310:ASN:O	2.17	0.45
1:C:325:ARG:HA	1:C:325:ARG:HD3	1.79	0.45
1:E:248:PHE:CZ	1:E:250:ALA:HA	2.51	0.45
1:A:28:THR:CG2	1:A:269:VAL:HG13	2.47	0.45
1:B:357:THR:HG22	1:B:358:HIS:ND1	2.32	0.45
1:C:73:ARG:HH12	1:C:92:HIS:CE1	2.35	0.45
1:E:260:ASN:HB2	1:E:261:LEU:HG	1.99	0.45
1:B:28:THR:CG2	1:B:269:VAL:HG11	2.47	0.45
1:C:295:TRP:HA	1:C:295:TRP:CE3	2.52	0.45
1:A:285:HIS:CD2	1:A:423:LEU:HD12	2.51	0.45
1:C:51:GLU:OE1	1:C:123:TYR:OH	2.33	0.45
1:E:153:THR:HG22	1:E:154:ALA:H	1.82	0.45
1:C:231:ARG:NH1	1:C:231:ARG:HG3	2.31	0.44
1:D:307:LEU:HD23	1:D:313:PRO:HA	1.98	0.44
1:F:256:ILE:CD1	1:F:264:VAL:HG12	2.47	0.44
1:B:195:VAL:HG21	1:B:206:LEU:CB	2.47	0.44
1:A:209:SER:HB2	1:A:233:PRO:HA	1.98	0.44
1:D:416:TYR:CE2	1:D:418:ALA:HB2	2.52	0.44
1:B:247:VAL:HB	1:B:255:LEU:HB2	1.98	0.44
1:B:308:ASP:O	1:B:309:GLN:C	2.61	0.44
1:D:69:TYR:O	1:D:120:HIS:HE1	2.00	0.44
1:C:392:GLY:C	1:C:394:GLU:H	2.26	0.44
1:D:214:PRO:HB3	1:D:231:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:TYR:CE1	1:F:143:PRO:HD2	2.52	0.44
1:B:316:ASN:OD1	1:B:318:ALA:HB3	2.17	0.44
1:F:2:MET:HA	1:F:6:GLU:OE2	2.18	0.44
1:F:22:LEU:HG	1:F:388:ALA:HB1	2.00	0.44
1:F:173:LEU:CD1	1:F:252:ALA:CA	2.92	0.44
1:F:258:PRO:HD3	1:F:402:SER:OG	2.18	0.44
1:A:180:ALA:HB1	1:E:107:SER:HB2	2.00	0.44
1:B:69:TYR:O	1:B:120:HIS:CE1	2.71	0.44
1:A:253:THR:OG1	1:A:267:ILE:HD12	2.18	0.44
1:F:66:MET:CG	1:F:122:ALA:HB2	2.47	0.44
1:A:250:ALA:HB1	1:A:251:PRO:HA	2.00	0.44
1:A:345:ALA:O	1:A:349:THR:HG23	2.17	0.44
1:B:69:TYR:O	1:B:120:HIS:HE1	2.01	0.44
1:D:3:THR:OG1	1:D:6:GLU:HG3	2.18	0.44
1:E:36:VAL:HG11	1:E:55:VAL:HG12	1.99	0.44
1:E:173:LEU:HD12	1:E:268:ASN:ND2	2.32	0.44
1:E:216:MET:HB3	1:E:366:LEU:HB3	2.00	0.44
1:E:245:SER:O	1:E:402:SER:HB2	2.18	0.44
1:A:378:ALA:HB1	1:A:389:ILE:HB	2.00	0.43
1:C:23:MET:HG2	1:C:251:PRO:HG2	1.99	0.43
1:D:131:MET:CE	1:D:281:ILE:HD11	2.48	0.43
1:F:42:THR:HA	1:F:43:PRO:HD3	1.92	0.43
1:B:67:ASP:HB3	1:B:120:HIS:CE1	2.53	0.43
1:B:247:VAL:HG11	1:B:400:VAL:CG1	2.48	0.43
1:E:81:ARG:NE	1:E:83:GLU:OE1	2.46	0.43
1:A:167:CYS:HB3	1:A:348:LEU:HD23	1.99	0.43
1:D:53:LEU:HA	1:D:66:MET:O	2.19	0.43
1:F:13:VAL:HG21	1:F:270:PRO:HB2	1.99	0.43
1:B:257:PRO:HA	1:B:258:PRO:HD2	1.88	0.43
1:C:356:ARG:HD3	1:C:372:ARG:NE	2.34	0.43
1:D:221:THR:HG23	1:D:225:PHE:HA	2.01	0.43
1:C:359:ASP:HB3	1:C:361:LEU:HD21	2.00	0.43
1:B:33:VAL:HG23	1:B:131:MET:C	2.43	0.43
1:B:250:ALA:HB1	1:B:251:PRO:HA	2.01	0.43
1:C:109:PRO:C	1:C:111:ALA:H	2.27	0.43
1:D:185:LEU:C	1:D:187:SER:H	2.27	0.43
1:E:291:GLU:O	1:E:292:THR:C	2.61	0.43
1:F:249:VAL:HB	1:F:253:THR:HB	1.99	0.43
1:B:203:LYS:O	1:B:204:THR:HB	2.19	0.43
1:E:28:THR:HG22	1:E:29:PRO:O	2.19	0.43
1:E:219:GLN:HE21	1:E:414:ARG:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:TYR:CD1	1:D:223:TYR:C	2.97	0.43
1:B:360:ARG:NH1	1:B:360:ARG:CG	2.78	0.43
1:C:8:GLU:OE2	1:C:12:ARG:NE	2.38	0.43
1:F:24:ARG:NH1	1:F:49:PHE:HB2	2.34	0.43
1:A:310:ASN:O	1:A:311:TYR:HB2	2.18	0.43
1:B:81:ARG:NH1	1:C:333:PHE:HA	2.34	0.43
1:C:365:ASP:O	1:C:369:VAL:HG23	2.19	0.43
1:D:176:ALA:HB2	1:D:266:ASN:ND2	2.34	0.43
1:D:360:ARG:CG	1:D:360:ARG:NH1	2.66	0.43
1:E:224:GLY:HA3	1:E:248:PHE:O	2.19	0.43
1:F:53:LEU:HA	1:F:66:MET:O	2.19	0.43
1:A:69:TYR:HB2	1:A:74:ARG:NH1	2.33	0.42
1:B:338:GLY:O	1:B:341:ASN:HB2	2.19	0.42
1:D:11:CYS:SG	1:D:356:ARG:NH1	2.92	0.42
1:D:250:ALA:HB1	1:D:251:PRO:HA	2.01	0.42
1:D:413:TRP:C	1:D:415:THR:N	2.74	0.42
1:E:215:ARG:HB2	1:E:230:LEU:HB2	2.00	0.42
1:D:292:THR:O	1:D:295:TRP:HB3	2.19	0.42
1:C:66:MET:HE3	1:C:120:HIS:HD2	1.84	0.42
1:E:79:TYR:O	1:E:90:LEU:HD11	2.20	0.42
1:F:156:THR:HG21	1:F:283:TRP:HE3	1.84	0.42
1:F:208:PRO:HD2	1:F:242:TYR:CZ	2.54	0.42
1:B:109:PRO:C	1:B:111:ALA:N	2.77	0.42
1:D:22:LEU:HG	1:D:388:ALA:HB1	2.01	0.42
1:A:55:VAL:HA	1:A:64:GLY:O	2.19	0.42
1:D:157:ARG:HA	5:D:602:HOH:O	2.18	0.42
1:E:147:PRO:O	1:E:397:THR:HG22	2.19	0.42
1:E:173:LEU:HD12	1:E:268:ASN:HD22	1.84	0.42
1:E:223:TYR:CG	1:E:396:ALA:HB2	2.54	0.42
1:F:226:ARG:HH21	1:F:403:PHE:HE2	1.68	0.42
1:A:79:TYR:CE2	1:D:349:THR:HG21	2.54	0.42
1:B:114:MET:O	1:B:118:VAL:HG23	2.18	0.42
1:B:357:THR:HG22	1:B:358:HIS:CE1	2.54	0.42
1:C:66:MET:CG	1:C:122:ALA:HB2	2.50	0.42
1:D:328:MET:HA	1:D:332:ASN:O	2.19	0.42
1:F:167:CYS:SG	1:F:172:ILE:HD11	2.60	0.42
1:F:260:ASN:OD1	1:F:260:ASN:N	2.52	0.42
1:B:192:PRO:CB	1:B:210:THR:HG22	2.50	0.42
1:D:77:LEU:HB3	1:D:87:LEU:HD21	2.01	0.42
1:F:72:HIS:HB3	3:F:502:FES:S2	2.60	0.42
1:F:293:GLU:OE1	1:F:293:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ALA:C	1:E:112:SER:N	2.78	0.42
1:E:162:LYS:HD2	1:E:279:TYR:CE1	2.55	0.42
1:E:230:LEU:HD23	1:E:243:VAL:HG22	2.00	0.42
1:C:73:ARG:C	1:C:74:ARG:HG2	2.44	0.42
1:B:220:ARG:HD3	1:B:370:GLU:OE2	2.20	0.42
1:D:2:MET:HE2	1:D:2:MET:HB3	1.92	0.42
1:A:144:GLU:HG2	5:A:722:HOH:O	2.20	0.41
1:B:325:ARG:HD3	1:B:325:ARG:HA	1.59	0.41
1:C:315:ARG:HB3	1:C:321:PHE:HA	2.02	0.41
1:E:16:ASP:O	1:E:17:ALA:C	2.63	0.41
1:F:166:PRO:HD2	1:F:348:LEU:HD21	2.02	0.41
1:A:3:THR:N	1:A:6:GLU:OE2	2.50	0.41
1:D:346:MET:O	1:D:350:MET:HG3	2.20	0.41
1:B:263:ASN:HB2	1:B:283:TRP:CE2	2.55	0.41
1:B:292:THR:HG22	1:B:293:GLU:N	2.35	0.41
1:C:123:TYR:CD1	1:C:136:MET:HA	2.55	0.41
1:C:295:TRP:HA	1:C:295:TRP:HE3	1.86	0.41
1:B:145:PHE:CD2	1:B:145:PHE:C	2.98	0.41
1:B:249:VAL:HB	1:B:253:THR:HB	2.03	0.41
1:D:365:ASP:O	1:D:369:VAL:HG23	2.20	0.41
1:F:103:LEU:HD23	1:F:103:LEU:HA	1.88	0.41
1:A:220:ARG:H	1:A:220:ARG:HG2	1.62	0.41
1:B:94:TRP:CZ3	1:B:118:VAL:HG11	2.55	0.41
1:D:150:TRP:HA	1:D:283:TRP:CZ2	2.56	0.41
1:D:185:LEU:HD23	1:D:186:HIS:CE1	2.55	0.41
1:D:256:ILE:O	1:D:257:PRO:C	2.62	0.41
1:E:33:VAL:HG23	1:E:131:MET:C	2.45	0.41
1:F:209:SER:OG	1:F:211:ASP:HB3	2.21	0.41
1:C:173:LEU:HD13	1:C:252:ALA:CA	2.49	0.41
1:C:355:ASP:C	1:C:357:THR:H	2.29	0.41
1:C:42:THR:HA	1:C:43:PRO:HD3	1.93	0.41
1:C:77:LEU:HB3	1:C:87:LEU:HD21	2.02	0.41
1:F:30:ILE:O	1:F:31:CYS:HB3	2.20	0.41
1:F:332:ASN:HD22	1:F:333:PHE:N	2.19	0.41
1:B:355:ASP:C	1:B:357:THR:H	2.28	0.41
1:C:64:GLY:CA	1:C:98:VAL:HB	2.51	0.41
1:C:141:THR:O	1:C:143:PRO:HD3	2.20	0.41
1:C:250:ALA:HB1	1:C:251:PRO:HA	2.02	0.41
1:C:293:GLU:HB3	1:E:293:GLU:HB3	2.02	0.41
1:D:71:PRO:O	1:E:360:ARG:HB2	2.20	0.41
1:D:293:GLU:OE2	1:F:297:LYS:NZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ASP:HB3	1:E:415:THR:HB	2.03	0.41
1:A:22:LEU:HD23	1:A:23:MET:N	2.36	0.41
1:E:135:TYR:CE1	1:E:143:PRO:HD2	2.56	0.41
1:F:357:THR:HG22	1:F:358:HIS:CE1	2.56	0.41
1:A:351:GLY:O	1:A:352:PRO:C	2.64	0.40
1:B:200:ALA:HA	1:B:204:THR:O	2.21	0.40
1:C:97:ASP:O	1:C:98:VAL:C	2.60	0.40
1:F:23:MET:HE1	1:F:169:TRP:CE2	2.56	0.40
1:F:105:MET:HE3	1:F:115:VAL:HA	2.04	0.40
1:A:245:SER:O	1:A:402:SER:HB2	2.21	0.40
1:A:324:ASP:O	1:A:327:ALA:HB3	2.22	0.40
1:B:57:ARG:HA	1:B:62:ARG:O	2.21	0.40
1:B:326:ASN:O	1:B:329:LYS:N	2.54	0.40
1:C:3:THR:O	1:C:4:HIS:C	2.64	0.40
1:F:66:MET:HE3	1:F:120:HIS:HD2	1.85	0.40
1:F:138:PRO:O	1:F:139:LYS:C	2.63	0.40
1:F:221:THR:HB	1:F:222:GLY:H	1.78	0.40
1:C:18:PRO:HB3	1:C:383:GLU:HG3	2.03	0.40
1:D:13:VAL:HG21	1:D:270:PRO:HB2	2.03	0.40
1:D:68:GLU:HG3	1:D:78:VAL:HG23	2.04	0.40
1:D:113:GLY:HA2	5:D:617:HOH:O	2.21	0.40
1:F:184:SER:O	1:F:333:PHE:CD2	2.73	0.40
1:C:343:ASP:O	1:C:344:VAL:C	2.64	0.40
1:D:227:TYR:CE1	1:D:246:THR:HB	2.56	0.40
1:F:388:ALA:O	1:F:389:ILE:C	2.64	0.40
1:D:45:LYS:HB2	1:D:78:VAL:HG21	2.04	0.40
1:E:3:THR:O	1:E:4:HIS:C	2.65	0.40
1:F:157:ARG:HB2	1:F:286:PRO:HA	2.04	0.40
1:F:224:GLY:HA3	1:F:248:PHE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/439 (91%)	350 (88%)	41 (10%)	8 (2%)	6	23
1	B	423/439 (96%)	368 (87%)	45 (11%)	10 (2%)	4	20
1	C	403/439 (92%)	354 (88%)	44 (11%)	5 (1%)	10	34
1	D	398/439 (91%)	362 (91%)	30 (8%)	6 (2%)	8	30
1	E	403/439 (92%)	354 (88%)	43 (11%)	6 (2%)	8	30
1	F	402/439 (92%)	358 (89%)	31 (8%)	13 (3%)	3	16
All	All	2428/2634 (92%)	2146 (88%)	234 (10%)	48 (2%)	6	23

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ALA
1	B	199	LYS
1	B	200	ALA
1	D	236	ASN
1	E	152	PRO
1	F	152	PRO
1	F	238	ALA
1	A	352	PRO
1	A	383	GLU
1	C	72	HIS
1	C	74	ARG
1	C	112	SER
1	D	106	ALA
1	E	209	SER
1	E	419	HIS
1	F	15	GLY
1	F	58	ASP
1	F	74	ARG
1	F	110	ALA
1	F	383	GLU
1	B	196	ASP
1	D	72	HIS
1	D	152	PRO
1	D	422	TRP
1	F	72	HIS
1	A	121	THR
1	B	72	HIS
1	B	152	PRO
1	B	207	ARG
1	D	398	PRO

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Mol	Chain	Res	Type
1	E	74	ARG
1	F	272	ASP
1	F	389	ILE
1	A	74	ARG
1	A	106	ALA
1	B	109	PRO
1	B	195	VAL
1	F	286	PRO
1	A	152	PRO
1	A	389	ILE
1	B	356	ARG
1	C	286	PRO
1	C	338	GLY
1	A	17	ALA
1	F	177	ILE
1	E	13	VAL
1	E	393	VAL
1	F	147	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/363 (93%)	293 (87%)	43 (13%)	4	16
1	B	349/363 (96%)	312 (89%)	37 (11%)	6	24
1	C	336/363 (93%)	297 (88%)	39 (12%)	5	20
1	D	335/363 (92%)	296 (88%)	39 (12%)	5	20
1	E	336/363 (93%)	301 (90%)	35 (10%)	7	25
1	F	335/363 (92%)	304 (91%)	31 (9%)	8	29
All	All	2027/2178 (93%)	1803 (89%)	224 (11%)	6	22

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	21	ARG
1	A	22	LEU
1	A	25	ARG
1	A	38	GLU
1	A	54	VAL
1	A	59	SER
1	A	90	LEU
1	A	98	VAL
1	A	114	MET
1	A	115	VAL
1	A	121	THR
1	A	125	THR
1	A	139	LYS
1	A	140	GLU
1	A	153	THR
1	A	156	THR
1	A	160	ILE
1	A	181	HIS
1	A	183	SER
1	A	184	SER
1	A	190	MET
1	A	207	ARG
1	A	216	MET
1	A	220	ARG
1	A	231	ARG
1	A	234	LEU
1	A	256	ILE
1	A	263	ASN
1	A	267	ILE
1	A	297	LYS
1	A	302	THR
1	A	305	VAL
1	A	329	LYS
1	A	352	PRO
1	A	357	THR
1	A	360	ARG
1	A	393	VAL
1	A	400	VAL
1	A	407	VAL
1	A	411	THR
1	A	415	THR
1	A	423	LEU

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Mol	Chain	Res	Type
1	B	5	GLU
1	B	23	MET
1	B	45	LYS
1	B	54	VAL
1	B	73	ARG
1	B	91	TYR
1	B	98	VAL
1	B	103	LEU
1	B	114	MET
1	B	117	LYS
1	B	119	LYS
1	B	140	GLU
1	B	153	THR
1	B	173	LEU
1	B	183	SER
1	B	187	SER
1	B	190	MET
1	B	194	ARG
1	B	195	VAL
1	B	201	THR
1	B	218	VAL
1	B	239	GLU
1	B	263	ASN
1	B	267	ILE
1	B	292	THR
1	B	294	THR
1	B	297	LYS
1	B	305	VAL
1	B	314	LEU
1	B	325	ARG
1	B	348	LEU
1	B	357	THR
1	B	360	ARG
1	B	366	LEU
1	B	411	THR
1	B	415	THR
1	B	417	ASP
1	C	1	MET
1	C	34	GLU
1	C	54	VAL
1	C	91	TYR
1	C	98	VAL

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Mol	Chain	Res	Type
1	C	103	LEU
1	C	114	MET
1	C	116	ASP
1	C	117	LYS
1	C	147	PRO
1	C	153	THR
1	C	164	LEU
1	C	173	LEU
1	C	182	SER
1	C	183	SER
1	C	187	SER
1	C	190	MET
1	C	210	THR
1	C	216	MET
1	C	231	ARG
1	C	232	ARG
1	C	263	ASN
1	C	286	PRO
1	C	295	TRP
1	C	297	LYS
1	C	305	VAL
1	C	320	LYS
1	C	329	LYS
1	C	357	THR
1	C	360	ARG
1	C	369	VAL
1	C	383	GLU
1	C	389	ILE
1	C	393	VAL
1	C	397	THR
1	C	409	LYS
1	C	410	THR
1	C	411	THR
1	C	423	LEU
1	D	5	GLU
1	D	23	MET
1	D	28	THR
1	D	44	VAL
1	D	54	VAL
1	D	62	ARG
1	D	98	VAL
1	D	108	GLU

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Mol	Chain	Res	Type
1	D	125	THR
1	D	139	LYS
1	D	153	THR
1	D	156	THR
1	D	164	LEU
1	D	177	ILE
1	D	190	MET
1	D	207	ARG
1	D	210	THR
1	D	216	MET
1	D	218	VAL
1	D	227	TYR
1	D	231	ARG
1	D	234	LEU
1	D	236	ASN
1	D	260	ASN
1	D	263	ASN
1	D	267	ILE
1	D	305	VAL
1	D	314	LEU
1	D	334	THR
1	D	344	VAL
1	D	357	THR
1	D	360	ARG
1	D	389	ILE
1	D	397	THR
1	D	406	ILE
1	D	409	LYS
1	D	411	THR
1	D	415	THR
1	D	423	LEU
1	E	4	HIS
1	E	5	GLU
1	E	54	VAL
1	E	91	TYR
1	E	114	MET
1	E	115	VAL
1	E	117	LYS
1	E	125	THR
1	E	144	GLU
1	E	152	PRO
1	E	153	THR

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Mol	Chain	Res	Type
1	E	173	LEU
1	E	177	ILE
1	E	183	SER
1	E	187	SER
1	E	190	MET
1	E	234	LEU
1	E	239	GLU
1	E	243	VAL
1	E	260	ASN
1	E	263	ASN
1	E	266	ASN
1	E	267	ILE
1	E	305	VAL
1	E	320	LYS
1	E	329	LYS
1	E	357	THR
1	E	360	ARG
1	E	397	THR
1	E	399	THR
1	E	400	VAL
1	E	409	LYS
1	E	410	THR
1	E	411	THR
1	E	415	THR
1	F	16	ASP
1	F	32	LEU
1	F	54	VAL
1	F	62	ARG
1	F	114	MET
1	F	115	VAL
1	F	117	LYS
1	F	139	LYS
1	F	140	GLU
1	F	141	THR
1	F	144	GLU
1	F	147	PRO
1	F	153	THR
1	F	158	VAL
1	F	168	ASN
1	F	177	ILE
1	F	179	SER
1	F	210	THR

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Mol	Chain	Res	Type
1	F	232	ARG
1	F	260	ASN
1	F	263	ASN
1	F	267	ILE
1	F	302	THR
1	F	305	VAL
1	F	329	LYS
1	F	357	THR
1	F	360	ARG
1	F	389	ILE
1	F	409	LYS
1	F	415	THR
1	F	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	342	GLN
1	B	26	HIS
1	B	82	ASN
1	B	120	HIS
1	B	288	GLN
1	B	404	GLN
1	C	120	HIS
1	C	266	ASN
1	D	120	HIS
1	D	236	ASN
1	D	266	ASN
1	D	301	GLN
1	D	332	ASN
1	E	219	GLN
1	F	120	HIS
1	F	332	ASN
1	F	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FES	E	502	1	0,4,4	-	-	-		
3	FES	C	502	1	0,4,4	-	-	-		
4	UB7	B	503	-	12,12,12	1.52	2 (16%)	16,16,16	0.78	0
3	FES	D	502	1	0,4,4	-	-	-		
3	FES	A	602	1	0,4,4	-	-	-		
3	FES	F	502	1	0,4,4	-	-	-		
3	FES	B	502	1	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	E	502	1	-	-	0/1/1/1
3	FES	C	502	1	-	-	0/1/1/1
4	UB7	B	503	-	-	0/8/8/8	0/1/1/1
3	FES	D	502	1	-	-	0/1/1/1
3	FES	A	602	1	-	-	0/1/1/1
3	FES	F	502	1	-	-	0/1/1/1
3	FES	B	502	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	UB7	C03-C10	3.82	1.57	1.49
4	B	503	UB7	C06-C07	2.40	1.54	1.49

There are no bond angle outliers.

There are no chirality outliers.

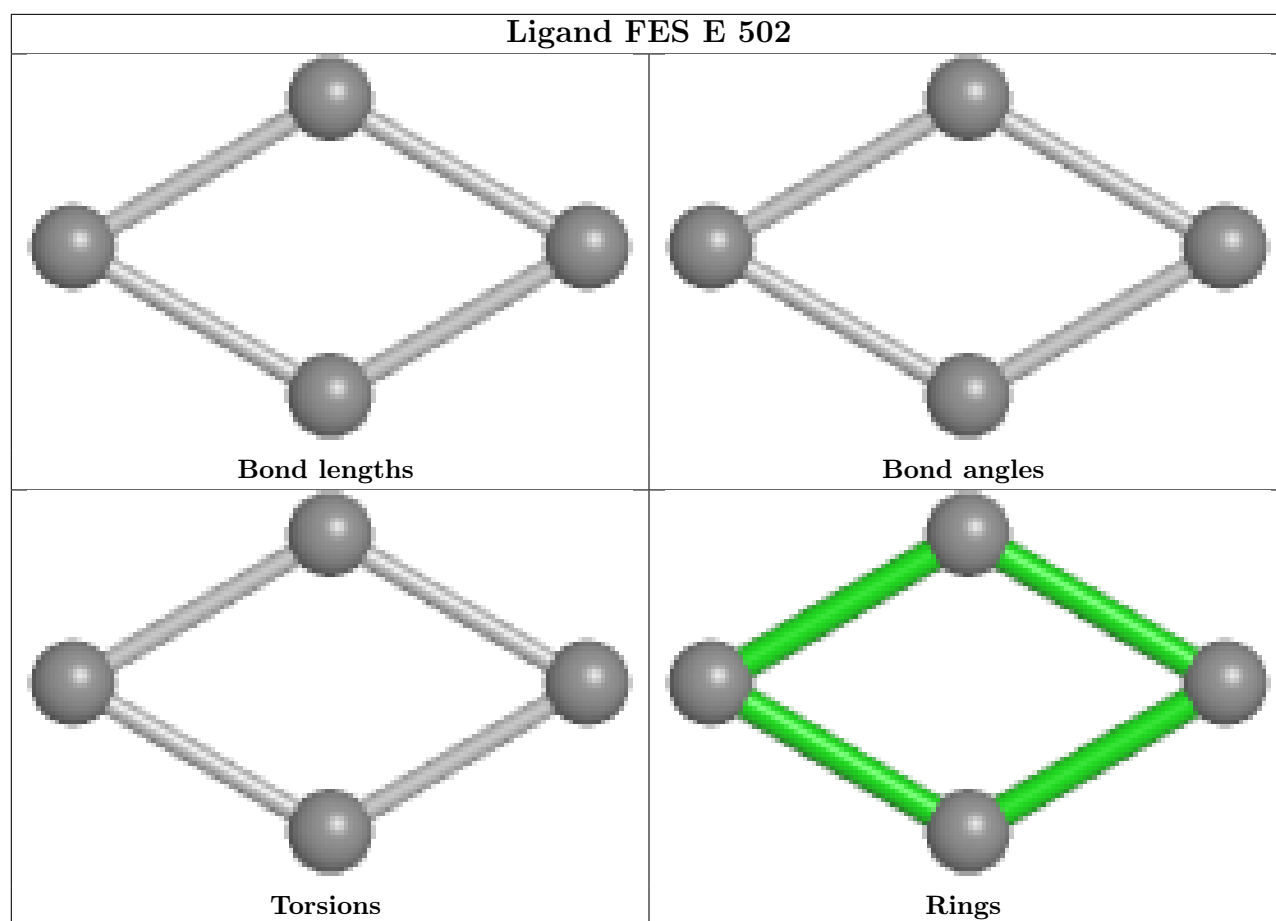
There are no torsion outliers.

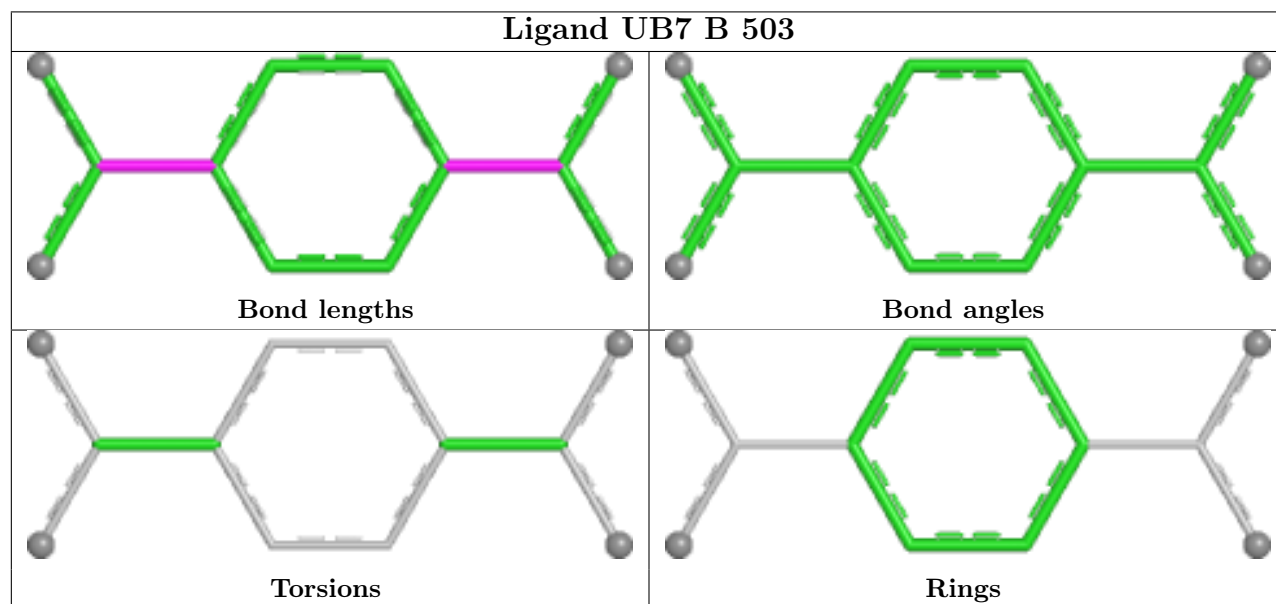
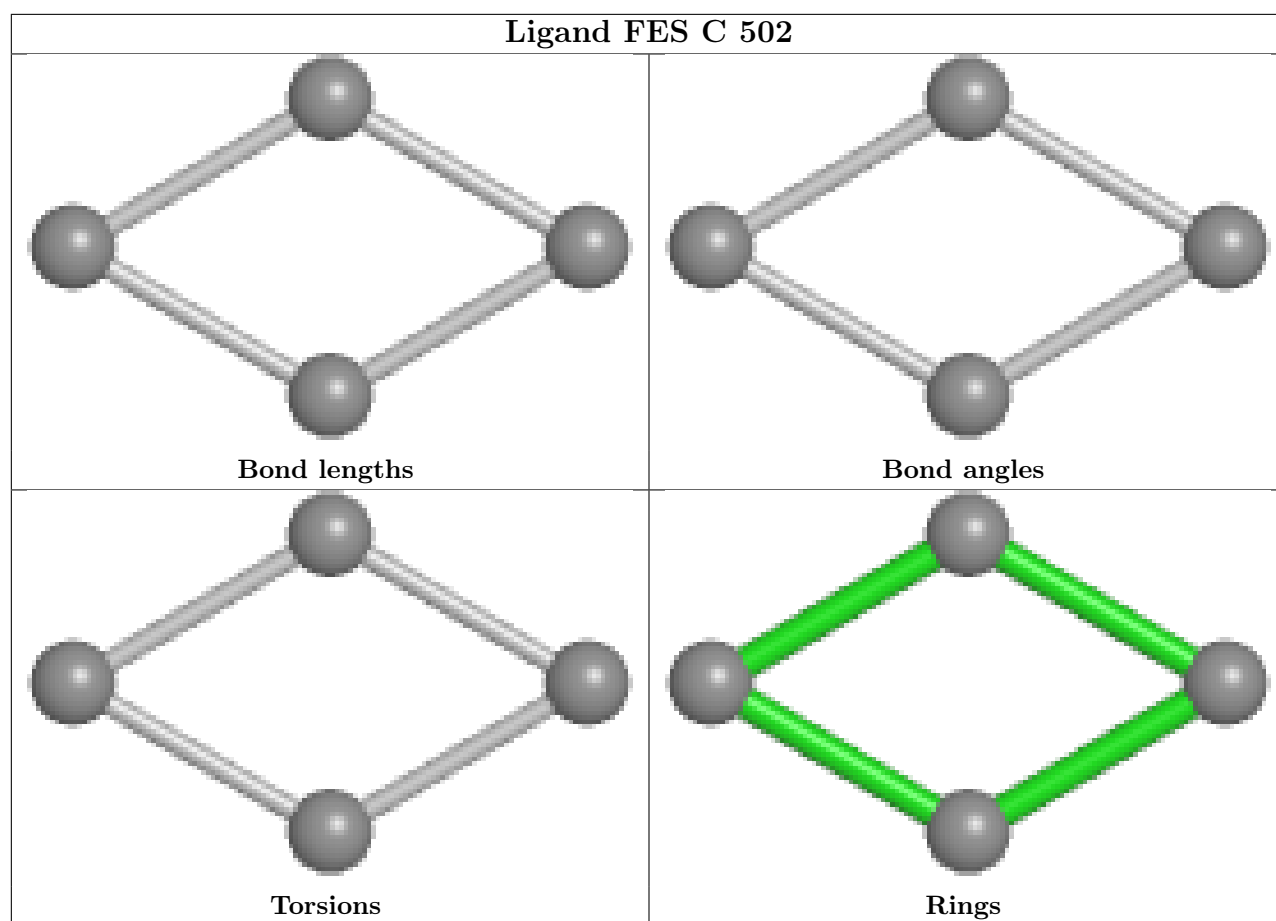
There are no ring outliers.

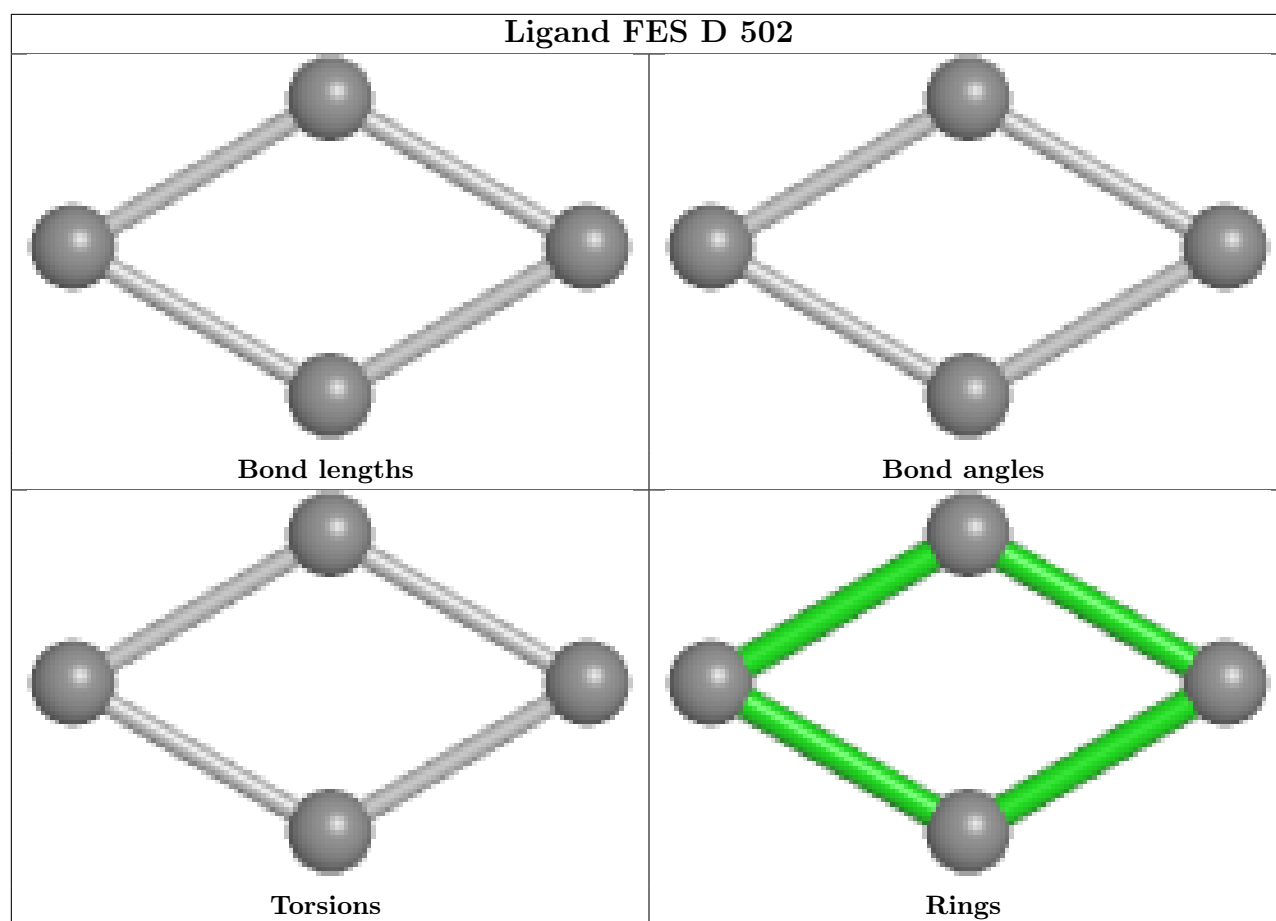
5 monomers are involved in 6 short contacts:

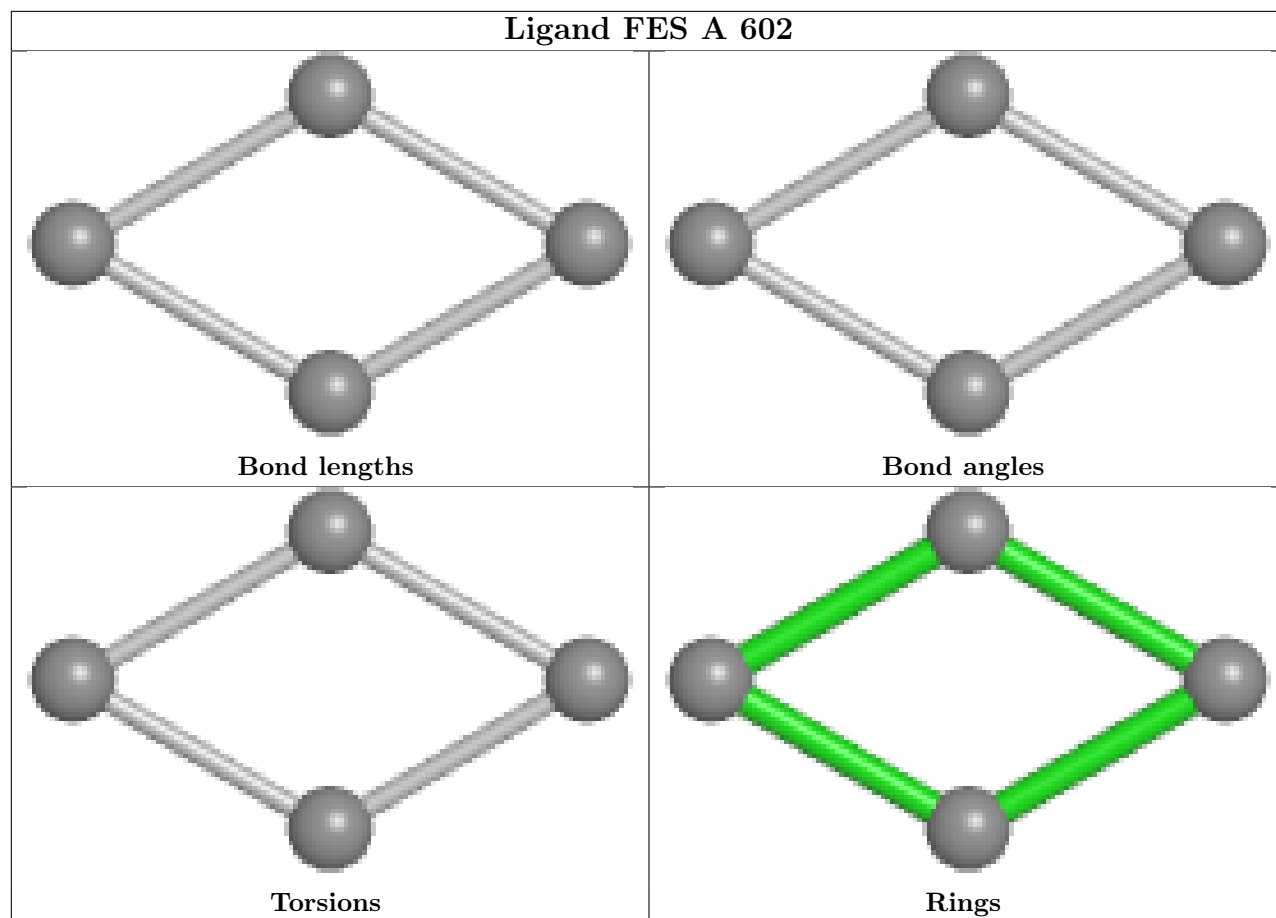
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	FES	1	0
3	C	502	FES	1	0
3	D	502	FES	2	0
3	F	502	FES	1	0
3	B	502	FES	1	0

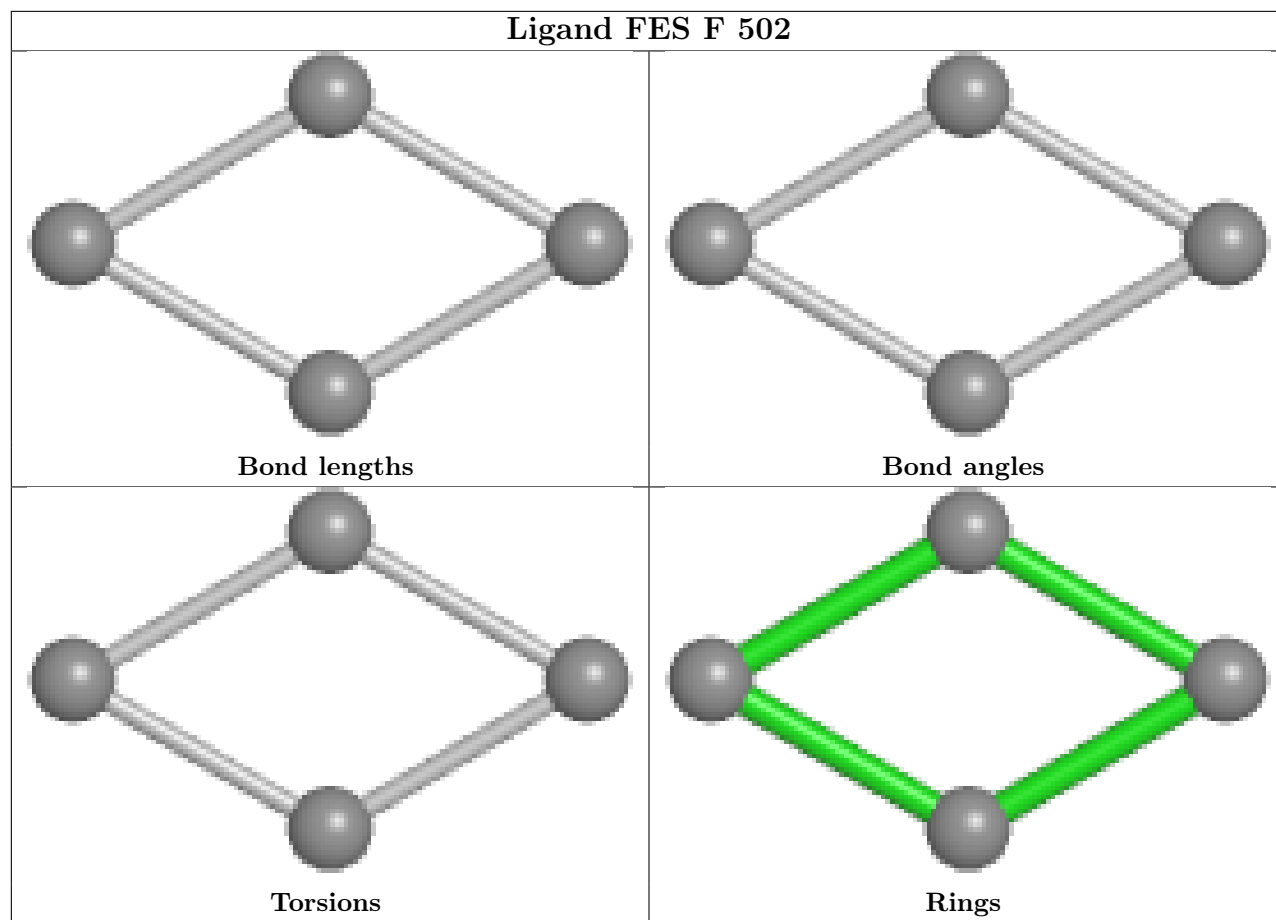
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

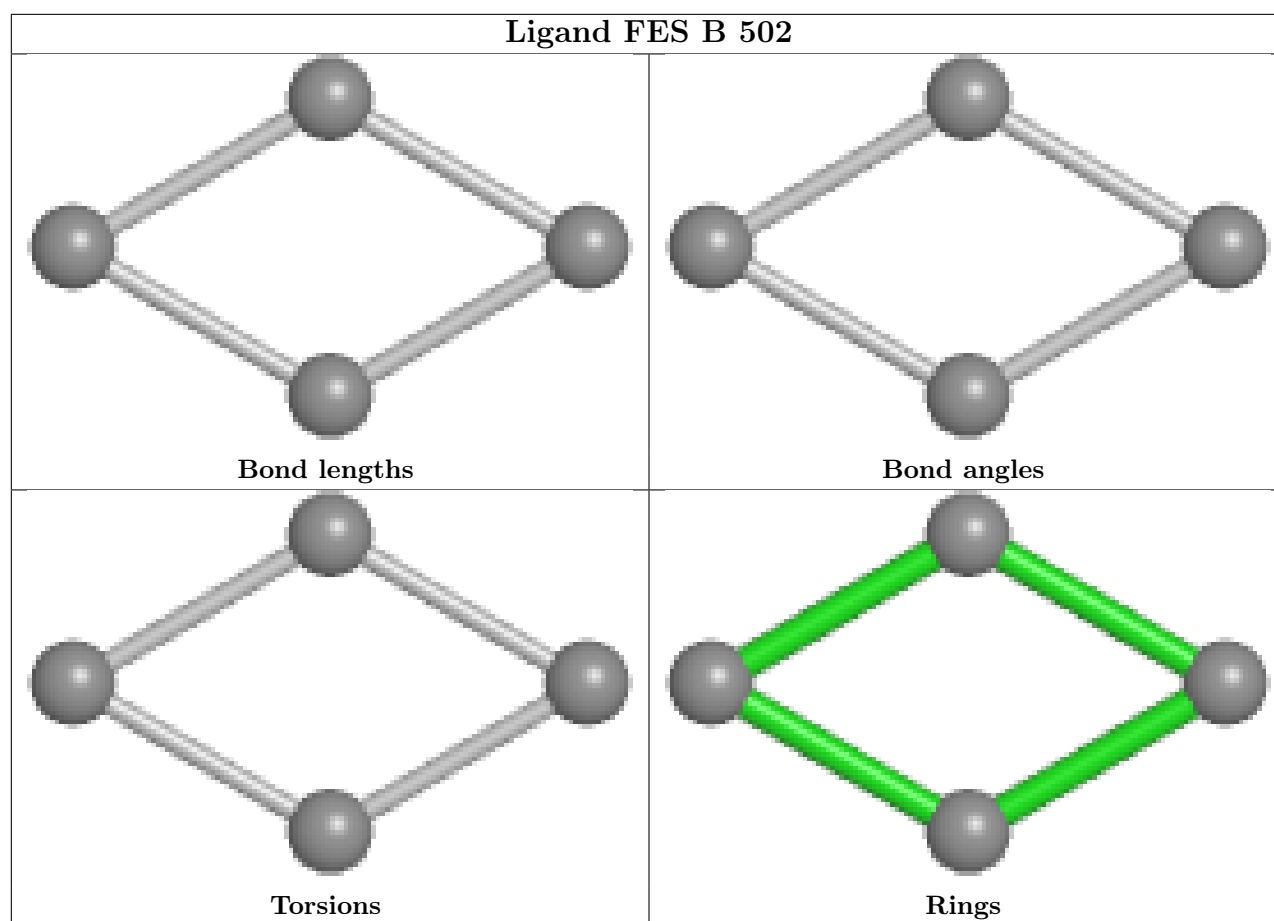












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	405/439 (92%)	0.31	18 (4%)	39 20	18, 35, 66, 108	0
1	B	425/439 (96%)	0.48	35 (8%)	17 9	17, 36, 85, 134	0
1	C	407/439 (92%)	0.41	29 (7%)	22 11	20, 36, 91, 186	0
1	D	404/439 (92%)	0.46	21 (5%)	33 17	19, 38, 75, 115	0
1	E	407/439 (92%)	0.77	68 (16%)	4 2	18, 39, 116, 142	0
1	F	406/439 (92%)	0.70	54 (13%)	7 4	22, 41, 95, 132	0
All	All	2454/2634 (93%)	0.52	225 (9%)	14 8	17, 37, 93, 186	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	MET	6.9
1	B	202	ASP	6.5
1	D	109	PRO	6.3
1	C	109	PRO	6.1
1	E	234	LEU	5.8
1	E	398	PRO	5.4
1	C	110	ALA	5.3
1	B	111	ALA	5.3
1	E	406	ILE	5.2
1	E	399	THR	5.1
1	C	411	THR	5.0
1	E	407	VAL	5.0
1	E	395	ALA	4.7
1	F	115	VAL	4.6
1	E	413	TRP	4.6
1	E	393	VAL	4.5
1	E	418	ALA	4.5
1	E	423	LEU	4.4
1	E	420	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	396	ALA	4.4
1	E	416	TYR	4.4
1	C	111	ALA	4.3
1	E	238	ALA	4.3
1	E	235	SER	4.3
1	D	154	ALA	4.3
1	E	213	ALA	4.3
1	E	400	VAL	4.3
1	F	406	ILE	4.2
1	C	115	VAL	4.1
1	F	214	PRO	4.1
1	B	109	PRO	4.1
1	D	108	GLU	4.1
1	C	112	SER	4.0
1	B	195	VAL	4.0
1	C	238	ALA	4.0
1	C	113	GLY	4.0
1	B	153	THR	4.0
1	E	208	PRO	3.9
1	F	237	ALA	3.9
1	E	216	MET	3.8
1	A	109	PRO	3.7
1	F	210	THR	3.7
1	E	419	HIS	3.7
1	D	113	GLY	3.7
1	E	421	VAL	3.7
1	F	234	LEU	3.6
1	F	154	ALA	3.6
1	B	108	GLU	3.6
1	E	397	THR	3.6
1	E	214	PRO	3.5
1	E	210	THR	3.5
1	F	209	SER	3.5
1	E	237	ALA	3.5
1	B	201	THR	3.5
1	B	110	ALA	3.5
1	B	204	THR	3.4
1	E	110	ALA	3.4
1	E	422	TRP	3.4
1	E	394	GLU	3.4
1	F	230	LEU	3.4
1	E	240	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	411	THR	3.4
1	E	405	ALA	3.4
1	E	415	THR	3.4
1	F	385	GLY	3.3
1	D	116	ASP	3.3
1	F	110	ALA	3.3
1	F	208	PRO	3.3
1	D	423	LEU	3.3
1	F	238	ALA	3.3
1	E	410	THR	3.2
1	A	190	MET	3.2
1	E	401	CYS	3.1
1	D	115	VAL	3.1
1	F	387	PRO	3.1
1	E	111	ALA	3.1
1	E	417	ASP	3.1
1	B	112	SER	3.1
1	E	227	TYR	3.1
1	D	237	ALA	3.1
1	C	139	LYS	3.1
1	A	107	SER	3.0
1	F	408	PRO	3.0
1	B	206	LEU	3.0
1	D	384	GLN	3.0
1	E	153	THR	3.0
1	C	237	ALA	3.0
1	E	207	ARG	3.0
1	F	416	TYR	3.0
1	F	407	VAL	3.0
1	F	236	ASN	3.0
1	C	234	LEU	2.9
1	B	115	VAL	2.9
1	D	155	ASP	2.9
1	B	239	GLU	2.9
1	E	109	PRO	2.9
1	F	111	ALA	2.9
1	F	107	SER	2.9
1	B	234	LEU	2.9
1	E	236	ASN	2.9
1	A	188	SER	2.9
1	B	114	MET	2.9
1	F	423	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	116	ASP	2.9
1	F	106	ALA	2.9
1	B	260	ASN	2.9
1	B	205	TRP	2.9
1	A	423	LEU	2.9
1	E	230	LEU	2.9
1	C	107	SER	2.8
1	E	154	ALA	2.8
1	F	398	PRO	2.8
1	A	411	THR	2.8
1	F	397	THR	2.8
1	F	393	VAL	2.8
1	E	212	LYS	2.8
1	B	113	GLY	2.8
1	E	408	PRO	2.8
1	F	213	ALA	2.8
1	A	115	VAL	2.8
1	E	364	SER	2.8
1	F	114	MET	2.7
1	F	153	THR	2.7
1	F	211	ASP	2.7
1	E	243	VAL	2.7
1	C	406	ILE	2.7
1	A	113	GLY	2.7
1	F	400	VAL	2.7
1	F	409	LYS	2.7
1	B	154	ALA	2.7
1	B	411	THR	2.7
1	D	107	SER	2.7
1	B	238	ALA	2.7
1	A	114	MET	2.6
1	D	190	MET	2.6
1	F	216	MET	2.6
1	F	399	THR	2.6
1	F	395	ALA	2.6
1	C	117	LYS	2.6
1	E	215	ARG	2.6
1	E	113	GLY	2.6
1	E	396	ALA	2.6
1	B	199	LYS	2.6
1	E	229	ALA	2.6
1	F	401	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	419	HIS	2.6
1	D	364	SER	2.5
1	C	154	ALA	2.5
1	C	1	MET	2.5
1	C	408	PRO	2.5
1	F	189	ASP	2.5
1	E	360	ARG	2.5
1	F	239	GLU	2.5
1	E	365	ASP	2.5
1	C	207	ARG	2.5
1	F	227	TYR	2.5
1	F	113	GLY	2.5
1	A	208	PRO	2.4
1	B	200	ALA	2.4
1	C	410	THR	2.4
1	B	4	HIS	2.4
1	F	212	LYS	2.4
1	E	223	TYR	2.4
1	C	219	GLN	2.4
1	E	209	SER	2.4
1	E	392	GLY	2.4
1	E	107	SER	2.4
1	E	114	MET	2.3
1	A	398	PRO	2.3
1	A	153	THR	2.3
1	F	363	ALA	2.3
1	C	146	LEU	2.3
1	F	417	ASP	2.3
1	A	396	ALA	2.3
1	E	412	ASP	2.3
1	E	414	ARG	2.3
1	C	106	ALA	2.3
1	A	415	THR	2.3
1	D	153	THR	2.3
1	F	235	SER	2.3
1	D	398	PRO	2.2
1	F	148	PRO	2.2
1	B	193	ALA	2.2
1	F	410	THR	2.2
1	C	420	TYR	2.2
1	A	338	GLY	2.2
1	E	409	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	217	GLN	2.2
1	D	114	MET	2.2
1	A	422	TRP	2.2
1	E	242	TYR	2.2
1	B	107	SER	2.2
1	C	190	MET	2.2
1	F	386	ALA	2.2
1	B	194	ARG	2.2
1	F	232	ARG	2.2
1	E	112	SER	2.2
1	B	190	MET	2.2
1	E	239	GLU	2.2
1	F	4	HIS	2.2
1	B	191	VAL	2.1
1	D	397	THR	2.1
1	C	233	PRO	2.1
1	F	109	PRO	2.1
1	F	422	TRP	2.1
1	F	364	SER	2.1
1	E	403	PHE	2.1
1	B	196	ASP	2.1
1	E	115	VAL	2.1
1	F	146	LEU	2.1
1	B	1	MET	2.1
1	B	229	ALA	2.1
1	D	106	ALA	2.1
1	A	239	GLU	2.1
1	C	208	PRO	2.1
1	D	152	PRO	2.1
1	A	318	ALA	2.1
1	C	236	ASN	2.1
1	D	118	VAL	2.0
1	E	188	SER	2.0
1	F	215	ARG	2.0
1	B	215	ARG	2.0
1	B	423	LEU	2.0
1	D	209	SER	2.0
1	E	285	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

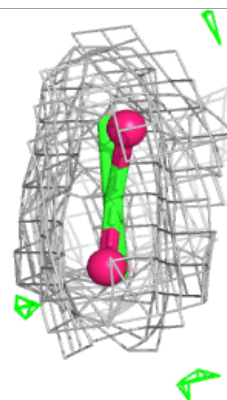
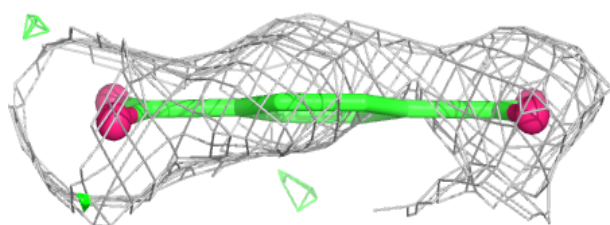
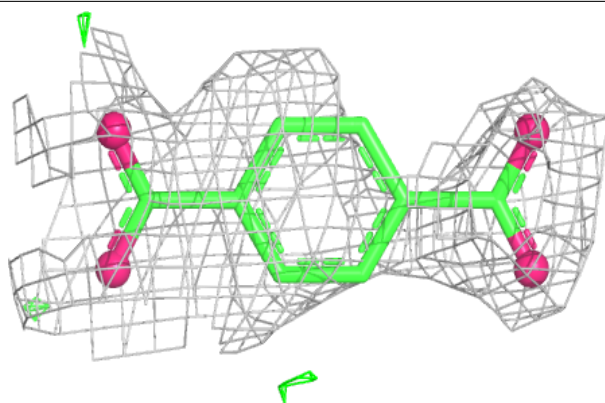
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UB7	B	503	12/12	0.85	0.25	61,75,89,89	0
3	FES	C	502	4/4	0.98	0.05	36,38,38,39	0
3	FES	E	502	4/4	0.98	0.04	20,21,24,25	0
2	FE2	E	501	1/1	0.98	0.04	23,23,23,23	0
2	FE2	A	601	1/1	0.99	0.02	16,16,16,16	0
2	FE2	F	501	1/1	0.99	0.03	26,26,26,26	0
3	FES	A	602	4/4	0.99	0.03	28,34,34,38	0
3	FES	B	502	4/4	0.99	0.03	26,28,30,32	0
2	FE2	B	501	1/1	0.99	0.03	29,29,29,29	0
3	FES	D	502	4/4	0.99	0.03	32,34,37,37	0
2	FE2	C	501	1/1	0.99	0.02	24,24,24,24	0
3	FES	F	502	4/4	0.99	0.04	31,32,35,36	0
2	FE2	D	501	1/1	0.99	0.03	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

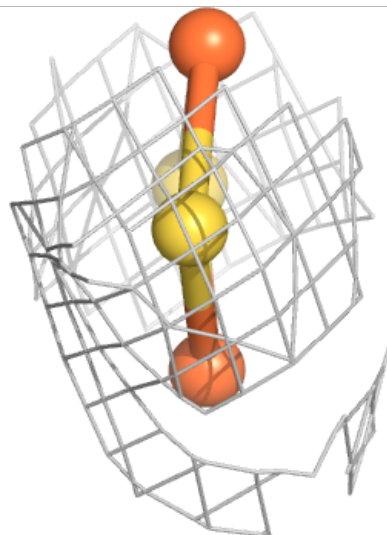
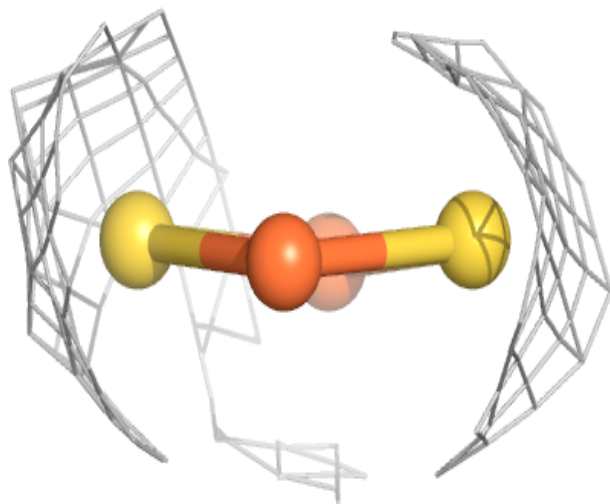
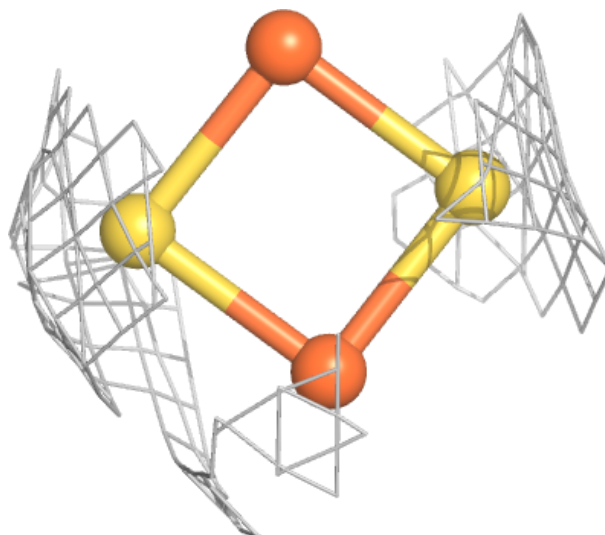
Electron density around UB7 B 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



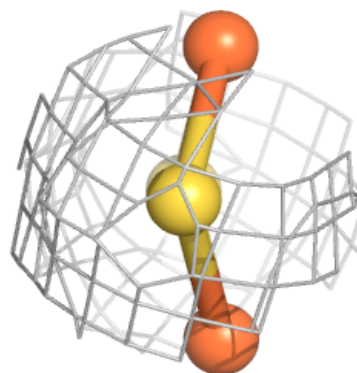
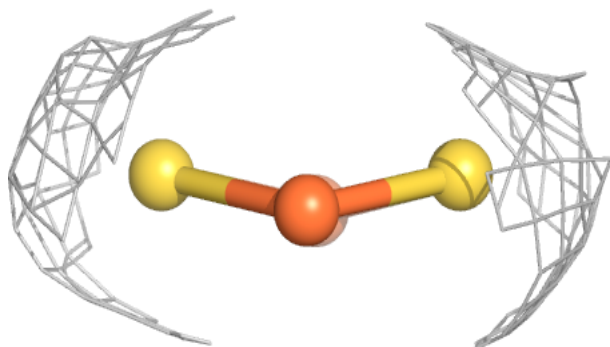
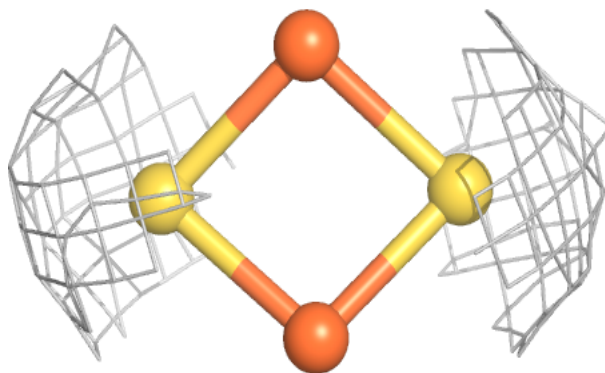
Electron density around FES C 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



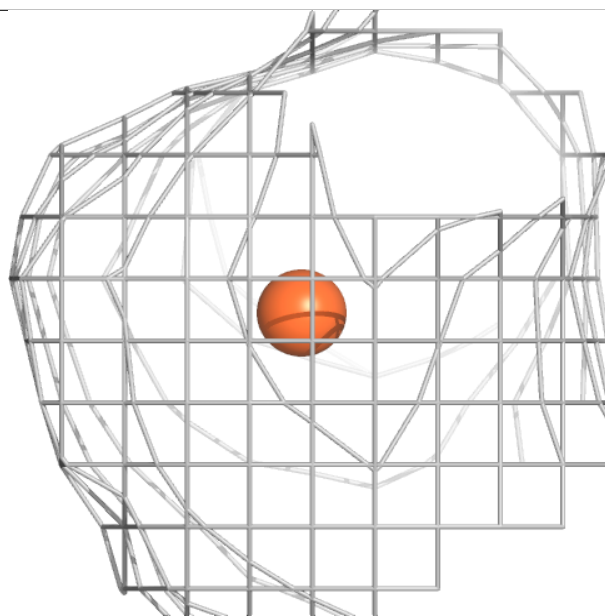
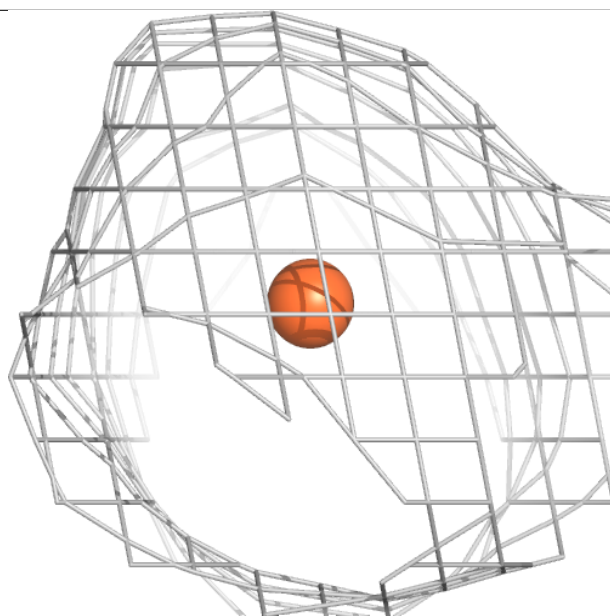
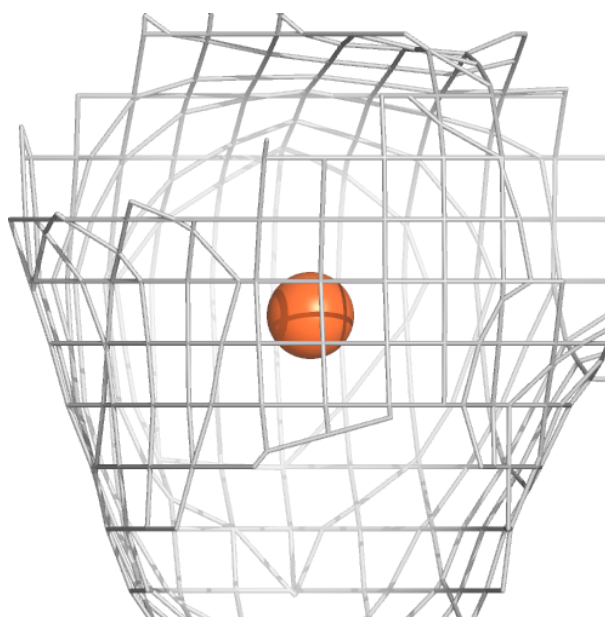
Electron density around FES E 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



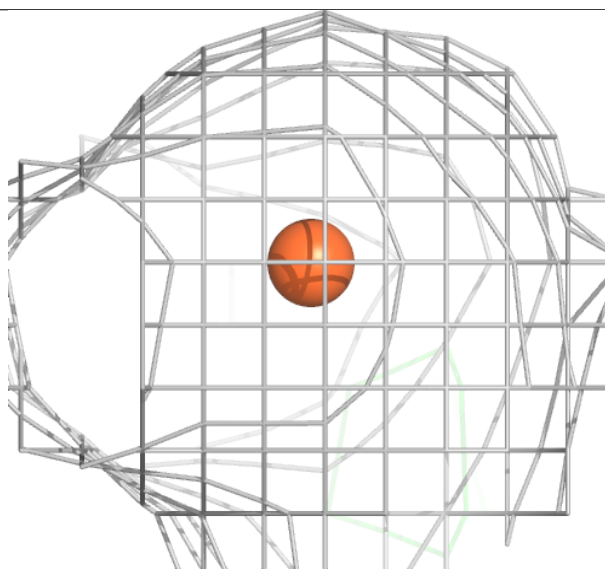
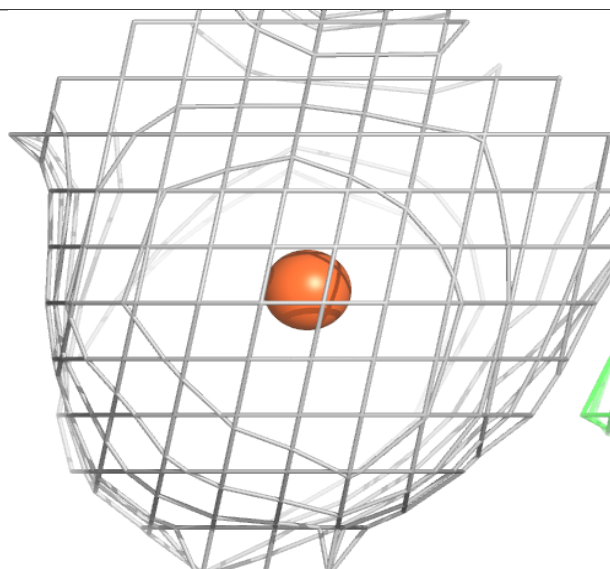
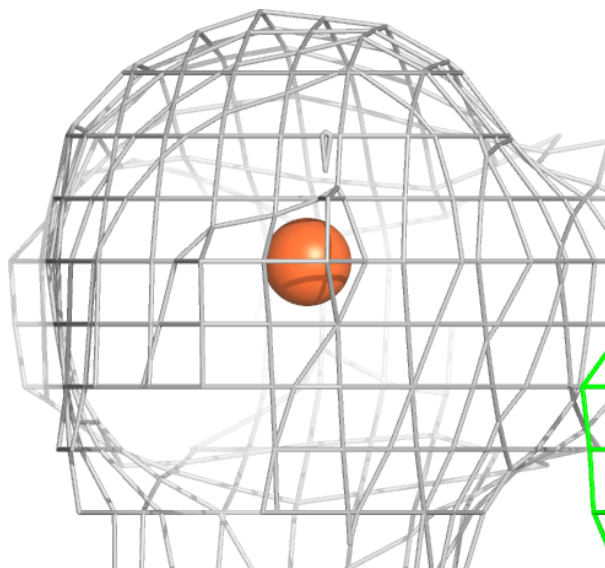
Electron density around FE2 E 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



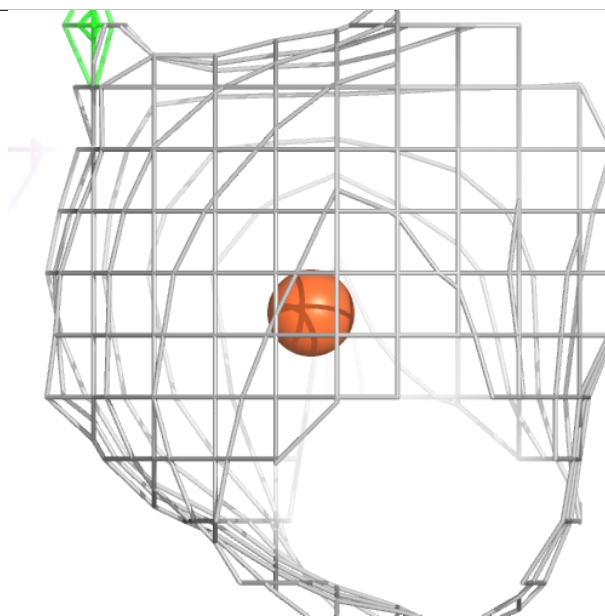
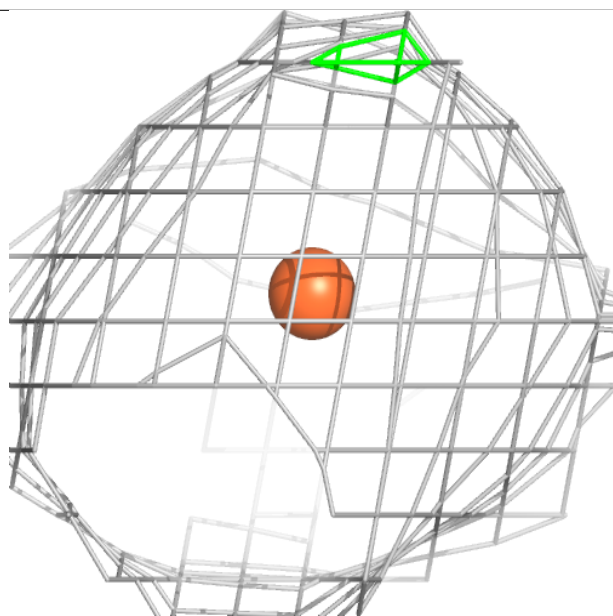
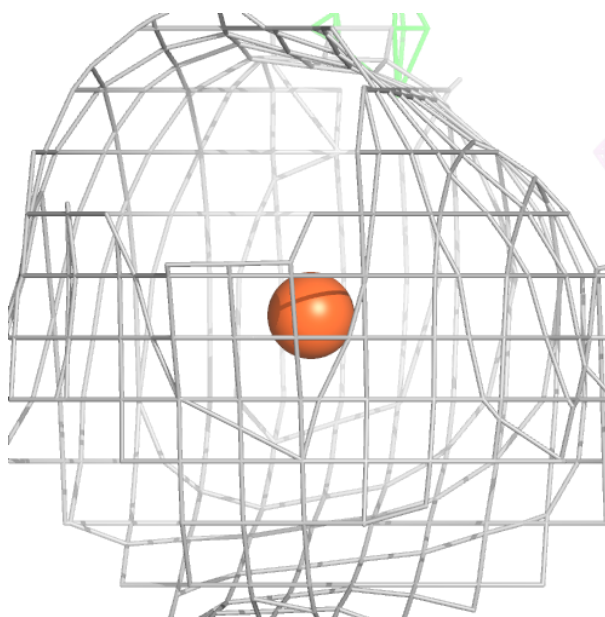
Electron density around FE2 A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



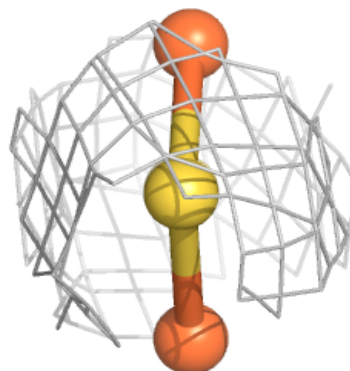
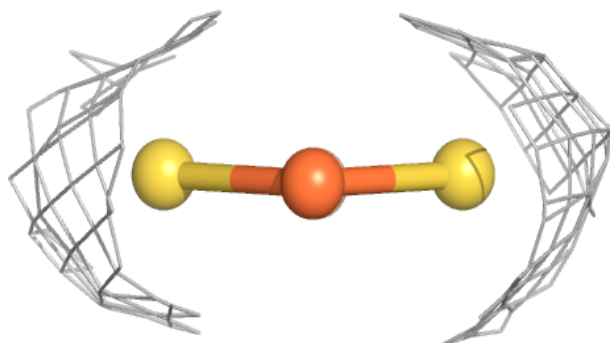
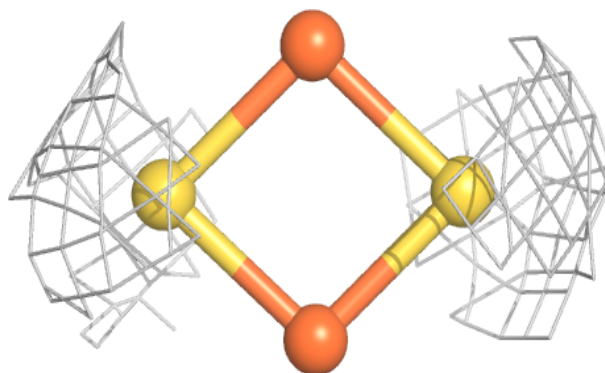
Electron density around FE2 F 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

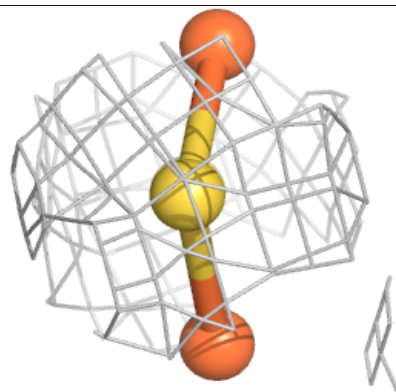
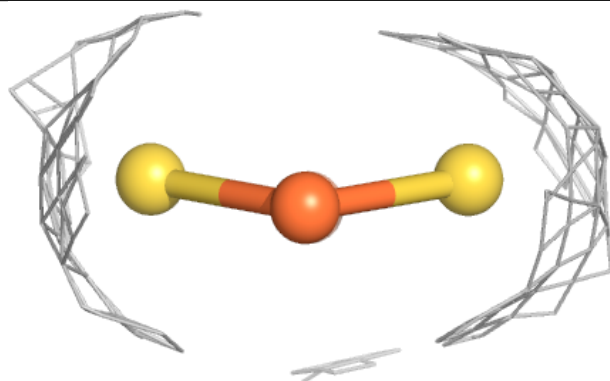
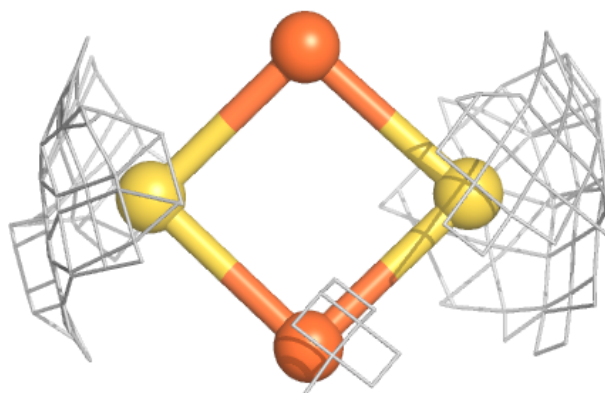


Electron density around FES A 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

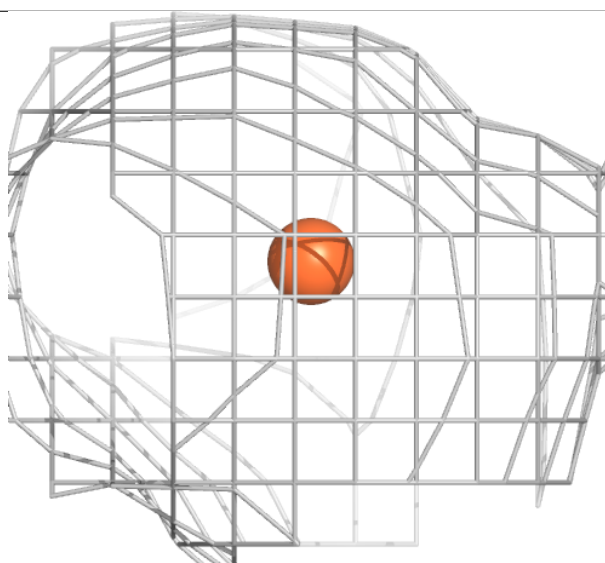
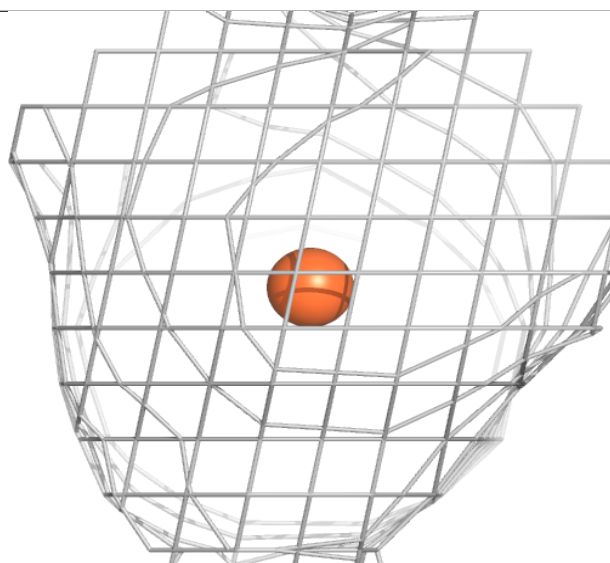
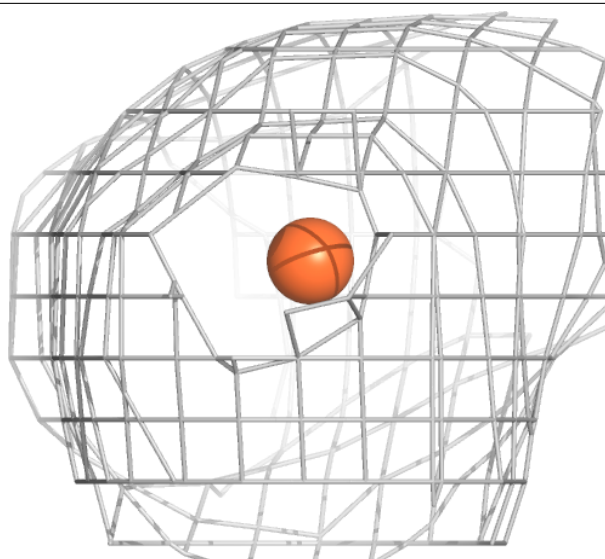
**Electron density around FES B 502:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



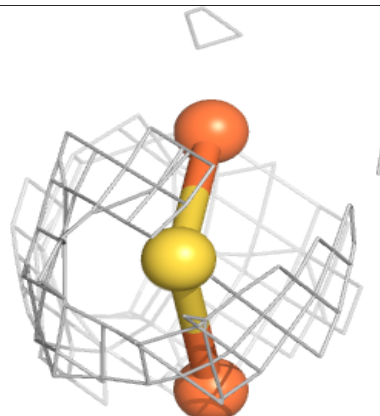
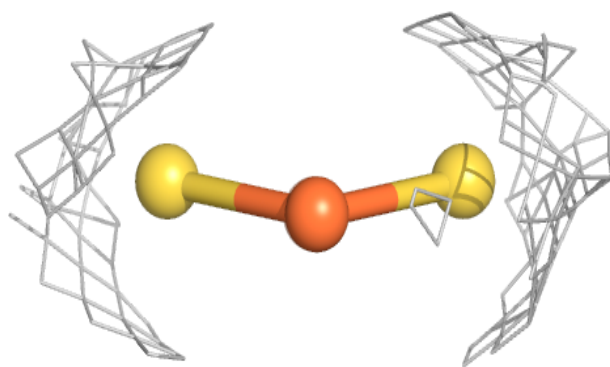
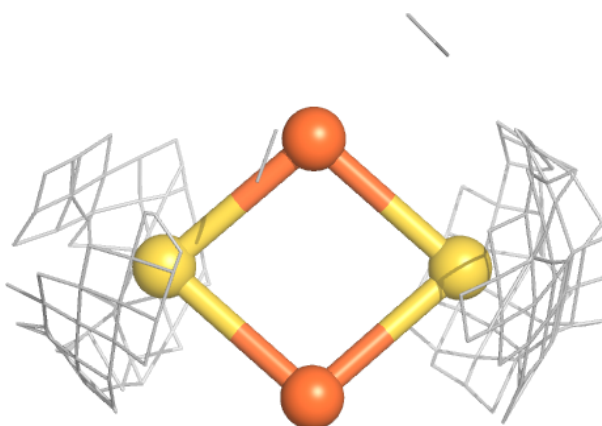
Electron density around FE2 B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



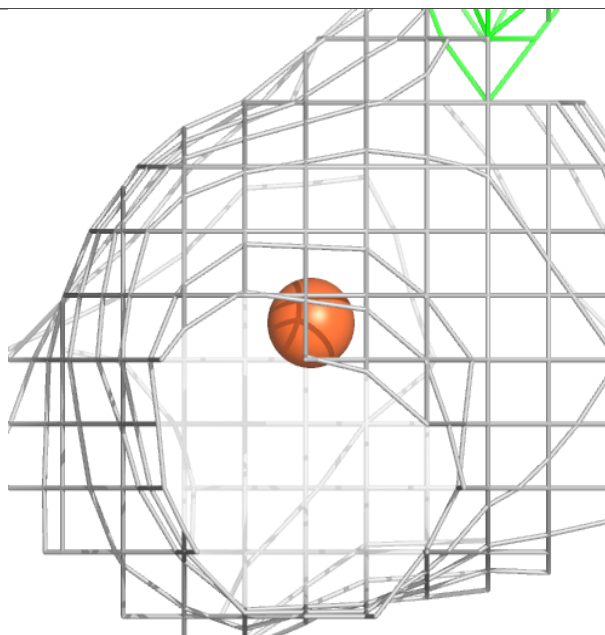
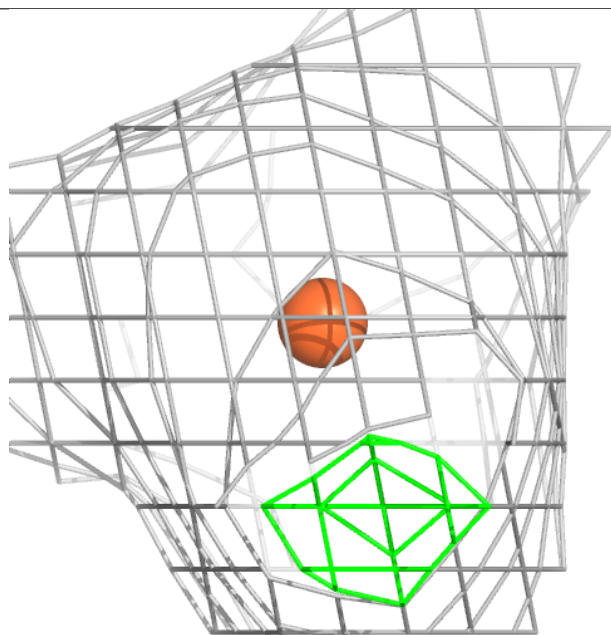
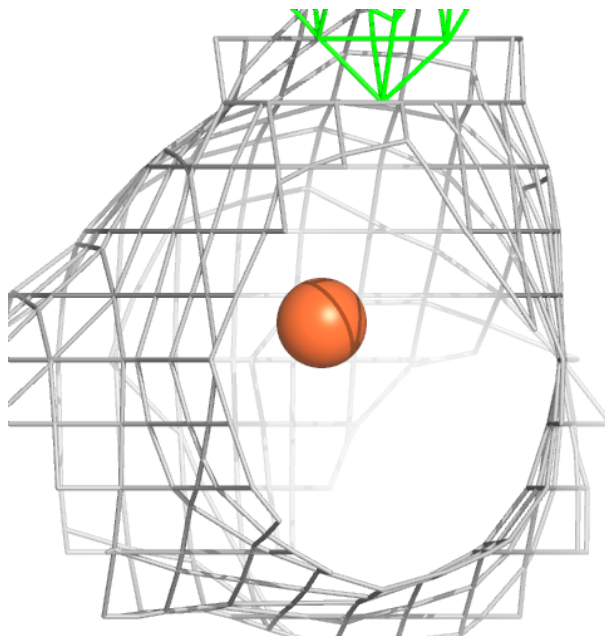
Electron density around FES D 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



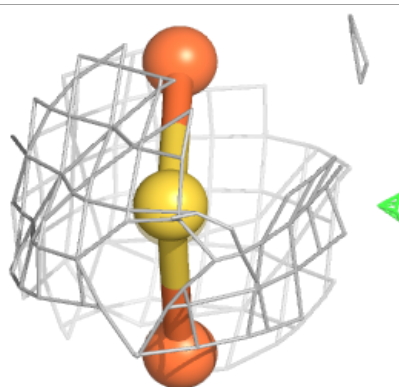
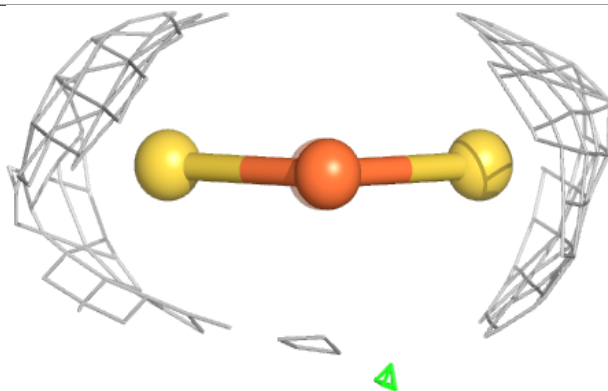
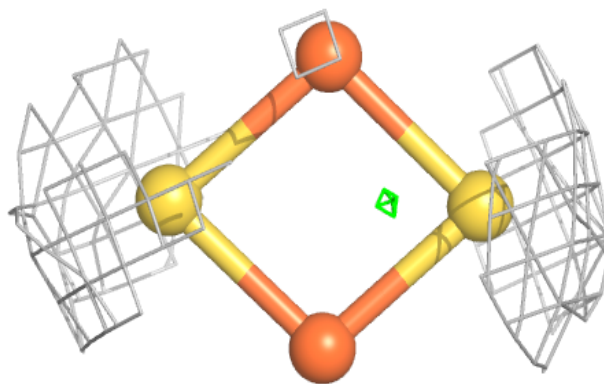
Electron density around FE2 C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



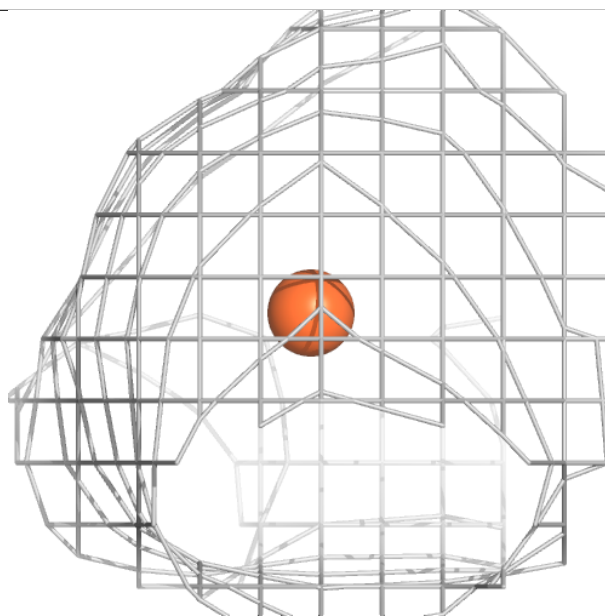
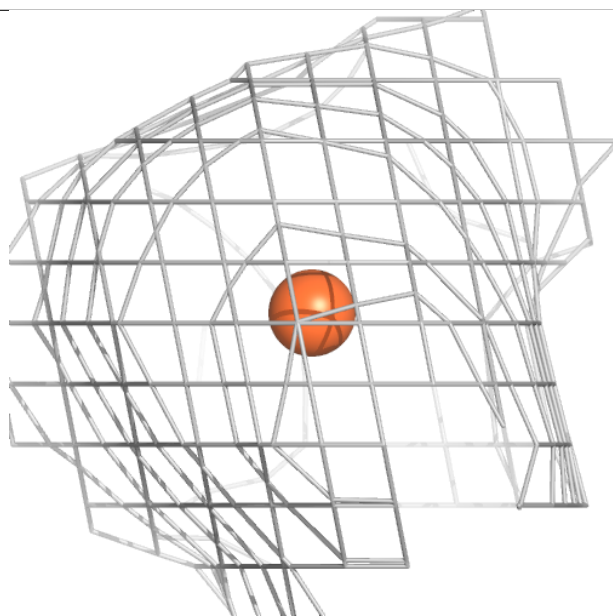
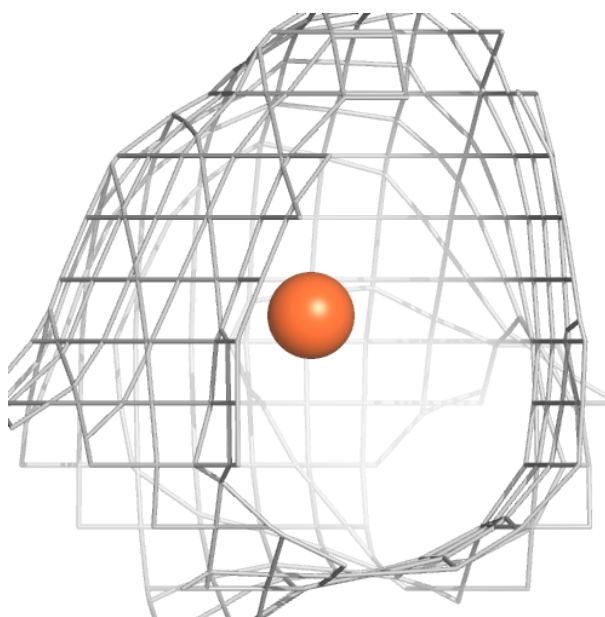
Electron density around FES F 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE2 D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.